

09/837, 745

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NEWS 15 OCT 28 BIOSIS file segment of TOXCENTER reloaded and enhanced

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MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
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FULL ESTIMATED COST	0.21	0.21

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STRUCTURE FILE UPDATES: 4 NOV 2003 HIGHEST RN 612801-40-8
DICTIONARY FILE UPDATES: 4 NOV 2003 HIGHEST RN 612801-40-8

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in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

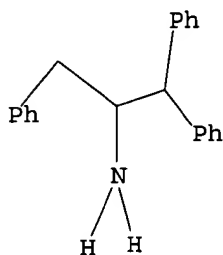
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Uploading 09857465.str

L1 STRUCTURE UPLOADED

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L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:38:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 117 TO ITERATE

100.0% PROCESSED 117 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 1692 TO 2988
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 16:38:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2356 TO ITERATE

100.0% PROCESSED 2356 ITERATIONS 22 ANSWERS
SEARCH TIME: 00.00.01

L3 22 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION

FULL ESTIMATED COST

148.15

148.36

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FILE COVERS 1907 - 5 Nov 2003 VOL 139 ISS 19
FILE LAST UPDATED: 4 Nov 2003 (20031104/ED)

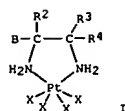
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 51 L3

=> d l4 30-51 abs ibib hitstr

L4 ANSWER 30 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
GI



AB The title complexes are described by the general formula I (B = a pR-C1-4 alkyl residue which may optionally have a R1 substituent in the Ph group with R1 = H, a halogen, a trihalomethyl, a C1-6 alkyl, a hydroxy, a C1-6 alkoxy, or a C2-6 alkanoyloxy group, in which B along with the H2N-CR2 segment forms a tetrahydroquinoline residue with B = benzyl, R2 = H, and with the CH2 group in the 2 position on the benzyl residue, in which

B along with the -CR2 segment forms a tetrahydronaphthyl residue in which 1 of the CH2 groups may be replaced by O, or in which B together with the -CR2 segment forms a decahydronaphthyl or indanyl residue: R2 = H, a C1-6 alkyl, a Ph, or a Ph-C1-4 alkyl group in which the Ph ring may be substituted with a halogen, hydroxy, C1-4 alkoxy, C1-4 alkyl, or C2-6 alkanoyloxy group; R3 and R4 are the same or different groups selected from H, C1-12 alkyl, C3-8 cycloalkyl, and (optionally C1-6 alkoxy-substituted) Ph groups; and X = H2O or a physiolog. acceptable anion; with the restriction that .gtoreq.1 of R2, R3, and R4 is not H

when B = a substituted or unsubstituted benzyl group. For Pt(II) complexes, 2 of the X's may be absent. Prepn. of the ligands entails redn. of selected precursors. Prepn. of the complexes entails reaction of a tetrahaloplatinic acid, a tetrahalo-Pt(II) complex, or a Pt(II) halide with the ligand or an acid addn. salt of the ligand, optionally oxidizing to produce a Pt(IV) compd., and exchanging any anions for physiolog. acceptable anions. Therapeutic agents (e.g., antitumor drugs) contg. the Pt complexes and methods for prep. them are also described.

ACCESSION NUMBER: 1993:51306 CAPLUS
DOCUMENT NUMBER: 118:51306
TITLE: Platinum complexes with phenylalkylethylenediamine ligands
INVENTOR(S): Brunner, Henri; Hankofer, Peter; Malterth, Friedrich; Engel, Juergen; Schumacher, Wolfgang; Hilgard, Peter; Voegel, Rainer
PATENT ASSIGNEE(S): Asta Pharma A.-G., Germany
SOURCE: Eur. Pat. Appl., 45 pp.
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 451753	A1	19911016	EP 1991-105514	19910408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 07112994	A2	19950502	JP 1991-69854	19910402

L4 ANSWER 31 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN

AB Optically active RICH:CR2CH(OH)CMe3 [I; R1 = (un)substituted C3-8 cycloalkyl, Ph; R2 = 1,2,4-triazol-1-yl], useful as fungicides, herbicides, and plant growth regulators (no data), were prep. by asym. redn. of a ketone RICH:CR2COCMe3 (II) with a borohydride modified with an optically active amino alc. R4NHCHRC3CR52OH [III; R3 = C1-8 alkyl, C7-11 aralkyl; R4 = H; R5 = H, (un)substituted C7-16 aralkyl, Ph]. Thus, a suspension of 0.551 g (5)-III.HCl (R3 = Me2CHCH2, R4 = H, R5 = Ph) in CH2Cl2 was cooled at 20.degree., a soln. of 0.0681 g NaBH4 in 1 mL DMF was added and the temp. of the mixt. was raised to room temp. over 2 h.

A soln. of 0.348 g (E)-II (R1 = 4-ClC6H4, R2 = 1,2,4-triazol-1-yl) in 4 mL ClCH2CH2Cl was added at room temp., the mixt. was stirred for 48 h, 6 mL 2NHCl was added and the stirring continued for 2 h to give 0.35 g of a mixt. contg. (+)-(E)-I (R1 = 4-ClC6H4, R2 = 1,2,4-triazol-1-yl) (78.9%) and (2)-I (20.3%), with a conversion of 96.3% (GC).

ACCESSION NUMBER: 1991:42792 CAPLUS
DOCUMENT NUMBER: 114:42792
TITLE: Method for producing an optically active azolyl-.alpha.,.beta.-unsaturated alcohol
INVENTOR(S): Yoneyoshi, Yukio; Suzukamo, Gohfu; Sakito, Yoji; Nishioka, Toshio
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: U.S., 8 pp. Cont.-in-part of U.S. Ser. No. 89,051, abandoned.
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4908455	A	19900313	US 1988-161242	19880219
WO 8504401	A1	19851010	WO 1984-JP162	19840403
W: DK, HU, US				
RW: BE, CH, DE, FR, GB, NL				
US 5698742	A	19971216	US 1993-87554	19930708

PRIORITY APPLN. INFO.: WO 1984-JP162 19840403
US 1984-682002 19841121
US 1987-89051 19870824
US 1988-161242 19880219
US 1989-454948 19891222
US 1992-897808 19920612

OTHER SOURCE(S): CASREACT 114:42792; MARPAT 114:42792

IT 130432-40-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. redn. with borohydride and, of unsatd. ketones, fungicides, herbicides, and plant growth regulators from)

RN 130432-40-5 CAPLUS
CN Benzeneopropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 30 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

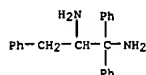
DE	1111249	A1	19920206	DE 1991-4111249	19910408
NO	9101373	A	19911011	NO 1991-1373	19910409
FI	9101698	A	19911011	FI 1991-1698	19910409
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HU	57788	A2	19911230	HU 1991-1145	19910409
ZA	9102630	A	19920129	ZA 1991-2630	19910409
CA	2040123	AA	19911011	CA 1991-2040123	19910410
US	5194644	A	19930316	US 1991-683431	19910410
NO	9204063	A	19911011	NO 1992-4063	19921020
NO	9204064	A	19911011	NO 1992-4064	19921020
US	5238955	A	19930824	US 1992-981475	19921125

PRIORITY APPLN. INFO.: DE 1990-4011520 19900410
NO 1991-1373 19910409
US 1991-683431 19910410

OTHER SOURCE(S): MARPAT 118:51306

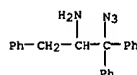
IT 126376-35-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 126376-35-0 CAPLUS
CN 1,2-Propanediamine, 1,1,3-triphenyl- (9CI) (CA INDEX NAME)

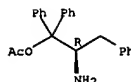


IT 126376-31-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in phenolalkylethylenediamine ligand prep.)

RN 126376-31-6 CAPLUS
CN Benzeneethanamine, .beta.-azido-.beta.-phenyl-.alpha.-(phenylmethyl)- (9CI) (CA INDEX NAME)

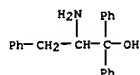


L4 ANSWER 31 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

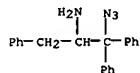


L4 ANSWER 32 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN
 AB p.cntdot.RC6H4CH2CR1(NH2)C(R2)2NH2 (L: R1 = H, R = Cl, R1 = Cl or R = H, R2 = Me, Et, cyclohexyl, 4-MeOC6H4, or R = MeO, R2 = 4-MeOC6H4; R = H, R2 = H, R1 = Ph, Me, Et, PhCH2) and PtCl2 were prepd. The chloride ligands of 4 complexes are replaced by the lactate anion. .alpha.-Cyclodextrin and polyvinylpyrrolidone are used to increase the water soly. of the Pt(II) complexes. The antitumor activity of the Pt(II) complexes is tested towards the P388 leukemia. The compds. with small alkyl substituents show antitumor activities which are much higher than the antitumor activity of cis-platinum. Compared to the insol. PtCl2, the lactate complexes and the formulations with .alpha.-cyclodextrin and polyvinylpyrrolidone exhibit good water soly., and no decrease of the antitumor activity is obsd.

ACCESSION NUMBER: 1990:244855 CAPLUS
 DOCUMENT NUMBER: 112:244855
 TITLE: Synthesis and antitumor activity of platinum(II) complexes of benzyl-1,2-diaminoethane ligands
 AUTHOR(S): Brunner, Henri; Hankofer, Peter; Treitinger, Barbara
 CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Regensburg, Regensburg, D-8400, Germany
 SOURCE: Chemische Berichte (1990), 123(5), 1029-38
 CODEN: CHBEAM; ISSN: 0009-2940
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 IT 57728-37-7P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and conversion of, to azide)
 RN 57728-37-7 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl- (9CI) (CA INDEX NAME)



IT 126376-31-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and redn. of, by aluminohydride)
 RN 126376-31-6 CAPLUS
 CN Benzenethanamine, .beta.-azido-.beta.-phenyl-.alpha.-(phenylmethyl)- (9CI) (CA INDEX NAME)

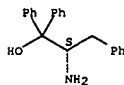


IT 126376-35-0P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 126376-35-0 CAPLUS
 CN 1,2-Propanediamine, 1,1,3-triphenyl- (9CI) (CA INDEX NAME)

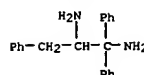
L4 ANSWER 33 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN
 AB A cross-linked polystyrene resin contg. chiral primary amino alc. moieties bound through the ether linkage to some of its p-methylene-substituted arom. rings is a useful regenerable chiral auxilliary in the enantioselective catalytic alkylation of aldehydes. The primary amino groups of the chiral amino alcs. reacts with the aldehydes to form Schiff bases, which catalyze the addn. of dialkylzinc to aldehydes leading to optically active secondary alcs. having enantiomeric purity of up to 99%. A series of polymeric amino alcs. were synthesized by two methods involving either attachment of a chiral moiety as a side chain onto a reactive cross-linked polystyrene, or the terpolymn. of a chiral monomer with styrene and a crosslinking agent. New crosslinking agents affording more flexibility to the chiral catalysts were used in the prepn. of the chiral polymers and found to provide excellent performance. An interesting extension of the method is its adaptation to a continuous-flow system where diethylzinc and aldehyde are supplied continuously to a column filled with the chiral polymeric catalyst. Large amts. of chiral products and high turnovers may be obtained by this method.

ACCESSION NUMBER: 1990:35375 CAPLUS
 DOCUMENT NUMBER: 112:35375
 TITLE: New solid-phase catalysts for asymmetric synthesis: cross-linked polymers containing a chiral Schiff base-zinc complex
 AUTHOR(S): Itsuno, Shinichi; Sakurai, Yoshiki; Ito, Koichi; Maruyama, Toshihiro; Nakahama, Seichi; Frechet, J. M.
 CORPORATE SOURCE: J. Sch. Mater. Sci., Toyohashi Univ. Technol., Toyohashi, 440, Japan
 SOURCE: Journal of Organic Chemistry (1990), 55(1), 304-10
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 112:35375
 IT 79868-78-3
 RL: RCT (Reactant); RACT (Reactant or reagent) (asym. alkylation of benzaldehyde with diethylzinc in presence of)
 RN 79868-78-3 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



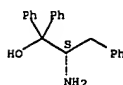
L4 ANSWER 32 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)



L4 ANSWER 34 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN
 AB A polymer-supported chiral amino alc. (I) was prepd. by the reaction of chloromethylated polystyrene and (S)-(-)-2-amino-3-(p-hydroxyphenyl)-1,1-diphenylpropan-1-ol; the chiral polymeric reagent was prepd. from I and borane. The asym. redns. of ketones and oxime ethers with the polymeric reagent were shown to give optically active alcs. and amines, resp. The results were compared with those obtained with (S)-(-)-2-amino-1,1,3-triphenylpropan-1-ol or (S)-(-)-2-amino-3-(p-benzyloxyphenyl)-1,1-diphenylpropan-1-ol, which are sol. model reagents.

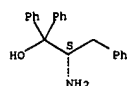
ACCESSION NUMBER: 1987:84089 CAPLUS
 DOCUMENT NUMBER: 106:84089
 TITLE: Asymmetric synthesis using chirally modified borohydrides. Part 4. Enantioselective reduction of ketones and oxime ethers with the reagent prepared from borane and polymer-supported
 (S)-(-)-2-amino-3-(p-hydroxyphenyl)-1,1-diphenylpropan-1-ol
 AUTHOR(S): Itsuno, Shinichi; Nakano, Michio; Ito, Koichi; Hirao, Akira; Owa, Masaki; Kanda, Naoki; Nakahama, Seichi
 CORPORATE SOURCE: Sch. Mater. Sci., Toyohashi Univ. Technol., Toyohashi, 440, Japan
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (12), 2615-19
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 106:84089
 IT 79868-78-3P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and stereoselective redn. of acetophenone oxime ethers by borane and)
 RN 79868-78-3 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 35 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB The asym. redn. of RCOPh (R = Me, Et, Pr, Bu), RCOMe (R = Bu, pentyl, hexyl, Me2CH, Me2CHCH2 Me3C), R1COCH2R2 (R1 = Ph, Me3C, R2 = Br, Cl), PhCOCH2OR3 (R3 = H, SiMe3, Ac), and PhMeC:NOR4, R4 = H, Me, Et, PhCH2, Me3Si, Ac) and R5MeC:NOMe (R5 = Ph, 1-, 2-naphthyl) by BH3 and (S)-H2NCHRA6CPh2OH (I, R6 = Me, Me2CH, Me2CHCH2, MeEtCH, PhCH2, MeSCH2CH2, 4-PhuCH2OC6H4CH2) or (R)-H2NCHPCPh2OH in THF took place with high enantioselectivity. I were prepd. from the resp. L-amino acid Me ester hydrochlorides by Grignard reaction with PhBr.
 ACCESSION NUMBER: 1987:18013 CAPLUS
 DOCUMENT NUMBER: 106:18013
 TITLE: Asymmetric synthesis using chirally modified borohydrides. Part 3. Enantioselective reduction of ketones and oxime ethers with reagents prepared from borane and chiral amino alcohols
 AUTHOR(S): Itsuno, Shinichi; Nakano, Michio; Miyazaki, Koji; Masuda, Hirofumi; Ito, Koichi; Hirao, Akira;
 Nakahama, Seiichi
 CORPORATE SOURCE: Sch. Mater. Sci., Toyohashi Univ. Technol., Toyohashi, 440, Japan
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (10), 2039-44
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 106:18013
 IT 79868-78-3P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and asym. redn. of ketones by borane and
 RN 79868-78-3 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha., .alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 36 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



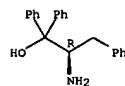
L4 ANSWER 36 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB RCH:CRICH(OH)CMe3 (I; R = cycloalkyl, cycloalkenyl, aryl, etc.; R1 = imidazol-1-yl, 1,2,4-triazol-1-yl) were prepd. by asym. redn. of ketones RCH:CRICOOMe3 (II) with metal borohydride agents modified by optically active R2CH(NHR3)C(R4)2OH (III; R2 = Cl-8 alkyl, C6-10 aryl, C7-11 aralkyl; R3 = H, Cl-6 alkyl, C7-16 aralkyl; R4 = H, Cl-10 alkyl, Ph, aralkyl, etc.). I were useful as fungicides, plant-growth regulators, and herbicides (no data). Thus, 1.8 mmol NaBH4 in DMF was added to a suspension of 1.8 mmol (S)-III HCl (R2 = Me2CHCH2, R3 = H, R4 = Ph) in ClCH2CH2Cl at -20.degree., followed by 1.2 mmol (E)-II (R = 4-ClC6H4, R1 = 1,2,4-triazol-1-yl), and the mixt. stirred at room temp. to give 0.35 g (+)-I (R = 4-ClC6H4, R1 = 1,2,4-triazol-1-yl), contg. 78.9% E- and 20.3% Z-isomer, with an optical yield of 72.2%.
 ACCESSION NUMBER: 1986:42462 CAPLUS
 DOCUMENT NUMBER: 105:42462
 TITLE: Optically active .alpha., .beta.-unsaturated alcohols
 INVENTOR(S): Komeyoshi, Yukio; Suzukamo, Gohfu; Sakito, Yoji; Nishioka, Toshio
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
 CODEN: JK00AF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61017567	A2	19860125	JP 1984-139799	19840704
JP 05028228	B4	19930423		

PRIORITY APPLN. INFO.: JP 1984-139799 19840704
 IT 103140-36-9
 RL: RCT (Reactant); RACT (Reactant or reagent) (modifier, for borohydride reducing agents)
 RN 103140-36-9 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha., .alpha.-diphenyl-, (R)-, acetate (salt) (9CI) (CA INDEX NAME)

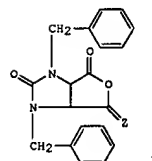
CH 1
 CRN 86906-05-0
 CMF C21 H21 N O

Absolute stereochemistry.



CH 2
 CRN 64-19-7
 CMF C2 H4 O2

L4 ANSWER 37 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 GI

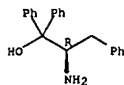


AB Optically active I (Z = H2), useful as an intermediate for optically active biotin, was prepd. by asym. redn. of I (Z = O) with B- or Al-contg. reducing agents modified with chiral alcs. or amines. Thus, 110 mg NaBH4 was stirred with 790 mg (S)-H2NCHMeCPh2OH.cntdot.HCl in CH2Cl2/DMF at 20-25.degree. for 1, 340mg cis-I (Z = O), and the resulting soln. stirred 2 h at 25.degree. to give 120 mg (3aS,6aR)-I (Z = H2).
 ACCESSION NUMBER: 1986:207262 CAPLUS
 DOCUMENT NUMBER: 104:207262
 TITLE: Optically active 1,3-dibenzylhexahydro-1H-furo[3,4-d]imidazole-2,4-dione
 INVENTOR(S): Ohashi, Naohito; Shimako, Kozo; Ishizumi, Kikuo
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JK00AF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60156691	A2	19850816	JP 1984-11453	19840125
JP 04032832	B4	19920601		

PRIORITY APPLN. INFO.: JP 1984-11453 19840125
 OTHER SOURCE(S): CASREACT 104:207262
 IT 100578-21-0
 RL: RCT (Reactant); RACT (Reactant or reagent) (asym. hydride redn. of imidazolidinedicarboxylic anhydride deriv. in presence of)
 RN 100578-21-0 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha., .alpha.-diphenyl-, hydrochloride, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L4 ANSWER 38 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB Optically active RICH:CR2CH(OH)CMe3 [I: R1 = (substituted)hydrocarbyl; R2 = imidazol-1-yl, 1,2,4-triazol-1-yl (Q)] were prepd. by asym. redn. of RICH:CR2COCMe3 (II) with a borohydride in the presence of an optically active amino alc. R4NHCHR3CR52OH [III: R3 = hydrocarbyl; R4 = H, hydrocarbyl; R5 = H, (substituted)hydrocarbyl]. Thus, a mixt. of 0.551 g (S)-III (R3 = Me2CHCH2, R4 = H, R5 = Ph).HCl, 0.0681 g NaBH4, and DMF was stirred at -20.degree. for 2 h, 0.348 g (E)-II (R1 = p-ClC6H4, R2 = Q) in ClCH2CH2Cl added at room temp., the mixt. stirred for 48 h, 6 mL 2N HCl added, and the mixt. stirred for 2 h to give (+)-(E)-I (R1 = p-ClC6H4, R2 = Q). I are useful as fungicides, herbicides, and plant growth

regulators

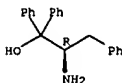
(no data).

ACCESSION NUMBER: 1986:109654 CAPLUS
 DOCUMENT NUMBER: 104:109654
 TITLE: Optically active .alpha.,.beta.-unsaturated alcohols
 INVENTOR(S): Yoneyoshi, Yukio; Suzukamo, Gohfu; Sakito, Yoji;
 Nishioka, Toshio
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 43 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8504401	A1	19851010	WO 1984-JP162	19840403
W: DK, HU, US				
RW: BE, CH, DE, FR, GB, NL				
EP 178325	A1	19860423	EP 1984-901412	19840403
EP 178325	B1	19920422		
R: BE, CH, DE, FR, GB, LI, NL				
HU 38319	A2	19860528	HU 1984-1719	19840403
HU 196765	B	19890130		
DK 8405622	A	19851204	DK 1984-5622	19841127
DK 170375	B1	19950814		
US 4908455	A	19900313	US 1988-161242	19880219
US 5144071	A	19920901	US 1989-454948	19891222
PRIORITY APPLN. INFO.:			WO 1984-JP162	19840403
			US 1984-682002	19841121
			US 1987-89051	19870824

IT 86906-05-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asymmetry-inducing agent, for asym. redn. of unsatd. ketones)
 RN 86906-05-0 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.-R)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



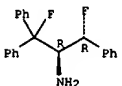
L4 ANSWER 39 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB Treatment of .alpha.,.beta.-amino alcs. with Olah's reagent (pyridine, 10HF) gave the corresponding .alpha.,.beta.-fluoro amines. E.g., reaction of PhC(OH)MeCMe2NH2 with Olah's reagent in CH2Cl2 at 20.degree. for 48 h gave 82% PhCFMeCMe2NH2. Fluoro hydroxy amines, fluoroaziridines, and difluoro amines were prepd. by the action of this reagent on .alpha.-hydroxy aziridines.

ACCESSION NUMBER: 1984:103081 CAPLUS
 DOCUMENT NUMBER: 100:103081
 TITLE: Fluorination of amino alcohols and hydroxyaziridines by Olah's reagent
 AUTHOR(S): Alverne, Gerard; Lacombe, Sylvie; Laurent, Andre; Rousset, Christine
 CORPORATE SOURCE: Equipe Rech., Univ. Claude Bernard Lyon I, Villeurbanne, F-69622, Fr.
 SOURCE: Journal of Chemical Research, Synopses (1983), (10), 246-7
 CODEN: JRPSDC; ISSN: 0308-2342
 DOCUMENT TYPE: Journal
 LANGUAGE: English/French
 OTHER SOURCE(S): CASREACT 100:103081

IT 88998-84-9P 88998-85-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

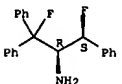
RN 88998-84-9 CAPLUS
 CN Benzenethanamine, .beta.-fluoro-.alpha.-(fluorophenylmethyl)-.beta.-phenyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 88998-85-0 CAPLUS
 CN Benzenethanamine, .beta.-fluoro-.alpha.-(fluorophenylmethyl)-.beta.-phenyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

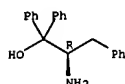


L4 ANSWER 40 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN
 AB Optically active RR1CHNCH2R2CR32OH [R, R1 = H, alkyl, Ph; R2 = alkyl, CH2Ph, Ph; R3 = CH2Ph, (un)substituted Ph] were prepd. Thus, (S)-H2NCHMeCPh2OH was N-formylated with HOAc-HCO2H to give (S)-HN(CHO)CHMeCPh2OH, which was reduced with LiAlH4 to (S)-MeNCHMeCPh2OH. These amino alcs. are reagents for asym. synthesis of compds. such as biotin.

ACCESSION NUMBER: 1983:504955 CAPLUS
 DOCUMENT NUMBER: 99:104955
 TITLE: Optically active amino alcohols
 INVENTOR(S): Aratani, Tadatoshi; Hazama, Motoo; Yoneyoshi, Yukio; Suzukamo, Gohfu
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
 SOURCE: Eur. Pat. Appl., 18 pp.
 CODEN: EPXKDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

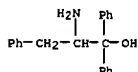
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 75868	A2	19830406	EP 1982-108806	19820923
EP 75868	A3	19830727		
R: BE, CH, DE, FR, GB, IT, LI				
JP 58052249	A2	19830328	JP 1981-151786	19810924
PRIORITY APPLN. INFO.:			JP 1981-151786	19810924
OTHER SOURCE(S):			CASREACT 99:104955	
IT 86906-05-0				
RL: RCT (Reactant); RACT (Reactant or reagent)				
(formylation of)				
RM 86906-05-0 CAPLUS				
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.-R)- (9CI)				
(CA INDEX NAME)				

Absolute stereochemistry.



L4 ANSWER 42 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN
 GI For diagram(s), see printed CA Issue.
 AB H2NCHRCR12OH (R = H, Me, CH2Ph, CHMe2, CH2CH2SMe, CH2CH2CR12OH; R1 = Et, Bu, Ph) were prepd. by treating H2NCHRCO2Et.HCl with 2-cyanocyclopentanone Na salt, Grignard reaction of the protected amino acids I, and cleavage of the protective group with 1.25N HCl.

ACCESSION NUMBER: 1976:31388 CAPLUS
 DOCUMENT NUMBER: 84:31388
 TITLE: Syntheses using 2-cyanocyclopentanone. Preparation of enamino esters. Application to the synthesis of .alpha.-amino alcohols
 AUTHOR(S): Lamant, Maurice; Guignard, Alain
 CORPORATE SOURCE: Lab. Synth. Org., Univ. Cathol. Ouest, Angers, Fr.
 SOURCE: Comptes Rendus des Seances de l'Academie des Sciences,
 Serie C: Sciences Chimiques (1975), 281(2-3), 123-6
 CODEN: CHDCAQ; ISSN: 0567-6541
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 IT 57728-37-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 57728-37-7 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl- (9CI) (CA INDEX NAME)



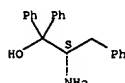
L4 ANSWER 41 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN
 AB H2NCHRCPh2OH [I, R = (S)-Me, (S)-CH2CHMe2, (S)-CH2Ph, and (R)-Ph] were prepd. by treating the corresponding H2NCHRCO2H with PhMgCl in THF.

Thus, a mixt. of PhMgCl (prepd. from 24.3 Mg and 40 g PhCl) and 12 g L-alanine in THF was refluxed 6 h to give 60% (S)-I (R = Me).

ACCESSION NUMBER: 1981:603530 CAPLUS
 DOCUMENT NUMBER: 95:203530
 TITLE: Optically active amino alcohols
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXKAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

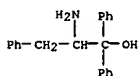
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56065847	A2	19810603	JP 1979-141666	19791031
JP 60016928	B4	19850430		
PRIORITY APPLN. INFO.:			JP 1979-141666	19791031
IT 79868-78-3P				
RL: SPN (Synthetic preparation); PREP (Preparation)				
(prepn. of)				
RN 79868-78-3 CAPLUS				
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.-S)- (9CI)				
(CA INDEX NAME)				

Absolute stereochemistry. Rotation (-).



L4 ANSWER 43 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN
 AB In order to find nonnarcotic analgesics, 54 amino tertiary alcs., in which a variety of substituents were involved at the C atom in 1-position and at the amino group, were synthesized by reacting various .alpha.- and .beta.-amino acid esters with Grignard reagents. These amino acid esters readily reacted with alkyl Grignard reagents to give the expected compds. However, when bulky aromatic Grignard reagents were reacted, the reactions stopped at the intermediate stage of formation of the corresponding ketones.

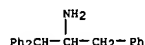
ACCESSION NUMBER: 1969:491836 CAPLUS
 DOCUMENT NUMBER: 71:91836
 TITLE: Application of amino acids as medicinal agents. I. Syntheses of the amino derivatives of tertiary alcohols
 AUTHOR(S): Hayashi, Seigoro; Furukawa, Mitsuru; Fujino, Yoko; Matsuishi, Naoto; Ohkawara, Tadashi
 CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1969), 17(1), 145-9
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 IT 23577-25-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 23577-25-5 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, hydrochloride (9CI) (CA INDEX NAME)



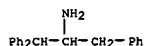
● HCl

L4 ANSWER 44 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB cf. CA 59, 15769f. The effects of Benzedrine (I), 1,3-diphenyl-2-aminopropane (II), 1,1-diphenyl-2-aminopropane (III), and 1,1,3-triphenyl-2-aminopropane (IV) were studied in mice and rabbits, singly and in conjunction with mephensin (V), chloral hydrate (VI), Amytal, Evipan, EtOH, Et2O, strychnine, and diazole. The min. effective dose required to produce stimulation was 2, 25, 20, and 4 mg./kg. for I, II, III, and IV, resp. I, II, III, and IV produced convulsive actions in mice when injected at doses equiv. to 1/2 L.D.50. II appeared to have a stronger effect than did III and IV. I had the mildest effects. I, II, III, and IV were generally antagonistic to the sleep-inducing, narcotic effects of V, VI, Amytal, Evipan, and EtOH. The duration of Et2O anesthesia was prolonged by I, II, and III while it was shortened by IV, however this required a dose equal to or greater than the L.D.50. I at 1/4 L.D.50 prolongs the latent period of strychnine action while III and IV shorten it. II could not be studied in this regard but did appear to be antagonistic to strychnine with respect to survival time. I, II, III, and IV shortened the latent period of diazole action. I and II were the strongest synergists while III and IV were somewhat weaker. Addnl. Ph groups do not qual. alter the action of I but do increase toxicity and restrict its therapeutic range.

ACCESSION NUMBER: 1963:484820 CAPLUS
 DOCUMENT NUMBER: 59:84820
 ORIGINAL REFERENCE NO.: 59:15769f-h
 TITLE: Structure-activity relation in the phenylisopropylamine group. III. Central activity of polyphenyl derivatives
 AUTHOR(S): Hano, Josef; Wojewodski, Wieslaw
 CORPORATE SOURCE: Polish Acad. Sci., Wroclaw, Pol.
 SOURCE: Arch. Immunol. Terapii Doswiadczalnej (1961), 9(4), 609-29
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 IT 94964-50-6, Phenethylamine, .alpha.-(diphenylmethyl)- (nervous system response to)
 RN 94964-50-6 CAPLUS
 CN Phenethylamine, .alpha.-(diphenylmethyl)- (7CI) (CA INDEX NAME)



L4 ANSWER 46 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB Unavailable
 ACCESSION NUMBER: 1963:484819 CAPLUS
 DOCUMENT NUMBER: 59:84819
 ORIGINAL REFERENCE NO.: 59:15769e-f
 TITLE: An analysis of the antiviral action of several drugs against Newcastle disease virus, vaccinia and, poliovirus in chicken embryo kidney and HeLa cells
 AUTHOR(S): Wright, Bruce Stewart
 CORPORATE SOURCE: Syracuse Univ., Syracuse, NY
 SOURCE: (1963) 155 pp. Avail.: Univ. Microfilms (Ann Arbor, Mich.), Order No. 63-3639
 DOCUMENT TYPE: Dissertation
 LANGUAGE: Unavailable
 IT 94964-59-7, Phenethylamine, .alpha.-(diphenylmethyl)-, hydrochloride (pharmacology of)
 RN 94964-59-7 CAPLUS
 CN Phenethylamine, .alpha.-(diphenylmethyl)-, hydrochloride (7CI) (CA INDEX NAME)

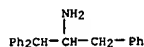


● HCl

L4 ANSWER 45 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB CA 55, 5873h. The pharmacol. actions of 1,3-diphenyl-2-aminopropane-HCl (I), 1,1-diphenyl-2-aminopropane-HCl (II), and 1,1,3-triphenyl-2-aminopropane-HCl (III) were studied. All 3 compds. are strong central stimulants, causing diminished anescompds. thetic effects in exptl. animals. Intravenous administration to rabbits and cats in amts. up to 1 mg./kg. produced increase in blood pressure, amts. 1-15 mg./kg. produced at first decrease followed by a long increase in blood pressure, and larger amts. caused a long lasting decrease in blood pressure. Atropine reduced the hypotensive effects without affecting the hypertensive ones. Expts. on isolated rabbit and frog hearts and cardioplethysmographic expts. showed detrimental effects of all compds. on the heart muscle.

The L.D.50 for white mice subcutaneously was 160, 64, and 12 mg./kg. for I, II, and III, resp. All 3 compds. are more toxic than amphetamine.

ACCESSION NUMBER: 1963:484820 CAPLUS
 DOCUMENT NUMBER: 59:84820
 ORIGINAL REFERENCE NO.: 59:15769f-h
 TITLE: Relation between chemical structure and pharmacological action in the phenylisopropylamine group. II. Aromatic derivatives
 AUTHOR(S): Hano, Josef; Wojewodski, Wieslaw
 CORPORATE SOURCE: Inst. Immunologii Terapii Doswiadczalnej PAN, Wroclaw, Pol.
 SOURCE: Arch. Immunol. Terapii Doswiadczalnej (1961), 9, 7-24
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 IT 94964-59-7, Phenethylamine, .alpha.-(diphenylmethyl)-, hydrochloride (pharmacology of)
 RN 94964-59-7 CAPLUS
 CN Phenethylamine, .alpha.-(diphenylmethyl)-, hydrochloride (7CI) (CA INDEX NAME)



● HCl

L4 ANSWER 47 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB There is described a new reaction between alkali metals and benzylamine which is apparently given by a whole series of amines. Intensely colored compds. are formed which in certain cases can be used for the quant. detection of the presence of certain organometallic compds. The results so far obtained are reported now because of the recent appearance of a paper by Stoelzel (C. A. 35, 7381.8). It had been shown (C. A. 33, 3761.7) that Ph2C:CHNH2 (I) can be obtained from Ph2C(OH)CH2NH2 (II) with concd. H2SO4, but the yield and purity of the product left much to be desired. In view of the extraordinary sensitivity of I to acids, it was attempted to effect the dehydration of II with a basic condensation agent.

When II in toluene was refluxed with powd. NaNH2 in the absence of moisture, the individual NaNH2 particles became in a few min. an intense cornflower-blue, the soln. itself remaining colorless. The color was discharged almost instantly by vigorous shaking with air, but under N it was stable. Under the same conditions Na and K instead of NaNH2 gave no color with II, but a no. of amino alcs. other than II and also simple amines (none of them purely aliphatic) do form colored reaction products with NaNH2 in the absence of moisture and air. The following colors were obtained: PhCH(OH)CH(NH2)Ph, red; Ph2C(OH)CH(NH2)CH2Ph, dirty red; PhCH2CH2NH2, yellowish red; PhCH2NH2, intense red; (PhCH2)2NH, brownish red; (PhCH2)3N, red; PhNH2, dark brown; Ph2NH, dark green; Ph3N, dark green; p-toluidine, violet; p-ClC6H4NH2, brown; o-O2NC6H4NH2, red; m-O2NC6H4NH2, green; pyridine, black-brown; piperidine, red-brown.

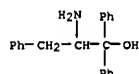
Although the color reaction is in general given by primary, secondary and tertiary aromatic and aromatic-aliphatic amines, it is possible that in individual cases the reaction of a tertiary and perhaps also of a secondary amine is due to preliminary cleavage to primary amines. The absorption spectra of the red solns. obtained from PhCH2NH2 and (PhCH2)2NH with NaNH2 were identical, but with Li instead of NaNH2 they were different. Furthermore, when (PhCH2)2NH in toluene was boiled 8 days with NaNH2 there was obtained, in addn. to unchanged (PhCH2)2NH, only 0.2 g. (PhCH2)2 and no PhCH2NH2 could be detected. K, even after shaking several days, does not react with II. Later expts. showed, however, that in general all alkali metals (and also organo-alkali compds.) react but the reaction velocity depends greatly both on the concn. of the amine and on the nature of the metal. To obtain as uncomplicated a picture as possible, PhCH2NH2 was chosen for further expts. The reaction with NaNH2 is strikingly accelerated by light, the color which appears in a few min. in daylight requiring several hrs. for its development in the dark. This sensitivity to light has thus far been observed only with NaNH2 and not with Na, K or Li. The products obtained with alkali metals and with NaNH2 gave with the Zeiss step photometer curves which showed no appreciable differences. All subsequent work was done with products obtained with Li,

which reacts about 10 times more rapidly than Na or K. The nature of the solvent plays but a subordinate role. A soln. of PhCH2NH2 in ether with Li under N in a sealed tube attained a max. of color in a few hrs., but after several hrs. longer the color distinctly diminished and in 24 hrs. the soln. had become completely colorless and a colorless cryst. ppt. had sepd. In one leg of each of 4 inverted U-shaped tubes was placed a PhCH2NH2-ether-Li mixt. and in the other leg ether, petr. ether, benzene and PhCH2NH2, resp., and the tubes were sealed under N. After the solns. in all 4 tubes had become colorless they were mixed with the solvents in the other leg of the tubes by tilting the tubes. In the first 3 tubes no change occurred whereas in the 4th tube the color was restored. The same

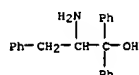
L4 ANSWER 47 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 as effect was obtained by mere warming of the colorless solns. It has not
 yet been possible to obtain the colored product in solid form for
 analysis. The colorless cryst. ppt., when removed from the N atm.,
 immediately becomes red and in a few sec. decomp. with evolution of
 fumes. The fine crystals were drawn off by suction under N from the
 coarse particles of unchanged Li through a fine tube, then collected on
 an asbestos filter, washed with ether, and dried a short time in vacuo under
 in N. The product so obtained, still moist with ether, contained N and Li
 the at. ratio 1:1. Decompn. with ice water gave PhCH2NH2 and NH3 in the
 mol. ratio 1:1, as detd. by distn. of the volatile bases with steam,
 conversion into the HCl salts, evapn. and extn. with abs. alc. The Li,
 NH3 and PhCH2NH2 contents left 13.6% unaccounted for, in all probability
 from due to ether still present in the original crystals. In the filtrate
 the crystals, after removal of the excess of PhCH2NH2 as carbamate, were
 identified BzOH (with PhCH2CO2H also present), one or more amines forming
 no solid product with CO2, BzH and (PhCH2)2. These results indicate that
 the primary reaction between PhCH2NH2 and Li must be very similar
 (PhCH2NH2 + 2Li → f.w.darw. PhCH2Li + LiNH2) to that between NH3 and alkali
 metals. To det. under what conditions the max. color intensity is
 obtained in the reaction, 10 and 2.5% solns. of PhCH2NH2 in ether were
 treated with from 1 to 1/24 equiv. of Li and the extinction coeffs. (at
 458 m.m.u.) of the mixts. were measured when the reactions had gone to
 completion (some days with the 10% soln., several weeks with the 2.5%
 soln.). The max. of extinction are obtained with a Li:PhCH2NH2 ratio of
 about 1:8 and are proportional to the concn. of PhCH2NH2. Although the
 substitution of Li for NaNH2 was already an improvement, its use still
 had considerable drawbacks from a preparative standpoint, and the readily
 available PhLi was accordingly investigated. This, too, gave a red soln.
 which on further addn. of PhLi was gradually decolorized and deposited a
 cryst. substance. This, however, was entirely different from that
 obtained with Li; it gave no evidence of great instability toward O and a
 soln. in PhCH2NH2 remained completely colorless; it dissolved easily in
 water without evolution of gas or any appreciable heat tone, m.
 106.degree. and had the compn. LiBr.2PhCH2NH2. On distn. in vacuo it
 gave pure PhCH2NH2 and left a residue of LiBr (originating from the PhLi
 soln. which had been prepd. from PhBr and Li in ether). Its structure was
 confirmed by synthesis from BuLi in benzene with PhCH2NH2.HBr and from
 PhCH2NH2.HBr in PhCH2NH2 with Li. Since the properties and method of
 prepn. of the red reaction product indicated it might be an ionized
 compd., cond. measurements were made under various conditions. In the
 mixt. of PhCH2NH2 and NaNH2 the appearance of the red color was
 accompanied by an appreciable cond. which disappeared with the
 decolorization of the soln. With Li the cond.-time curve had the same
 form as the curve obtained by plotting the extinction vs. the equivs. of
 Li (see above), showing clearly that the elec. cond. and color intensity
 are causally related. In measurements in which BuLi was dropped from a
 buret into PhCH2NH2 the cond., after reaching a max., decreased very
 slowly (because of the diln. by the ether of the BuLi soln.). The max.
 was dependent on the amt. of PhCH2NH2 and the concn. of the LiBu, lying
 usually in the neighborhood of 10 equivs. of LiBu; a further excess of
 LiBu had practically no effect. The curve obtained by adding PhCH2NH2 to
 BuLi was practically a straight line; a slight max. at the beginning of
 the curve (PhCH2NH2:LiBu = 1:1) may be due to the formation of an
 equimol.

L4 ANSWER 48 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB cf. C. A. 35, 7965.2. In continuation of the study on the relationship
 amines between chem. constitution and physiol. activity of sympathomimetic
 has derived from various ring systems, 1 deriv. of the phenanthrene series
 been synthesized and a no. of simple bases derived from benzene and the
 isoquinoline ring systems have also been prepd. for comparative
 pharmacol. study. Glycine ester-HCl (6.7 g.) and a soln. prepd. from 3.54 g. Mg,
 atm. 38.3 g. 9-bromophenanthrene and 100 cc. ether + 100 cc. benzene in an
 of dry H, when refluxed for 1 hr., cooled and decompd. with dil. HCl,
 yielded 2,2-bis(9-phenanthryl)-2-hydroxyethylamine-HCl, m. 239-40.degree.
 (decompn.); picrate, m. 209-10.degree. (decompn.). CH2BrCH2COCl, b30
 115-17.degree. (5 g.), from CH2BrCH2CO2H and SOCl2, on shaking with 5 g.
 homoveratrylamine (I) and dil. Na2CO3 soln. yielded 2.5 g.
 (.beta.-bromopropionyl)homoveratrylamine, m. 120-1.degree., which on
 of reaction with 10 g. POBr3 in 20 cc. CHCl3 for 1 week with the exclusion
 moisture, gave 0.4 g. 1-(2-bromomethyl)-3,4-dihydro-6,7-
 dimethoxyisoquinoline (II), thick brown oil; picrate, decomp. at
 166-8.degree.. Because of the low yield of II, the synthesis of
 1-(2-aminoethyl)-3,4-dihydro-6,7-dimethoxyisoquinoline was not attempted.
 o-(beta.-Bromopropionamido)biphenyl, m. 118.degree., was obtained in 50%
 soln. yield, but it failed to cyclize to 9-(2-bromoethyl)phenanthridine.
 Ph2CHCH2CONH2, m. 124-5.degree., obtained from Ph2CHCH2CO2H via the
 chloride, yielded Ph2CHCH2NH2.HCl, m. 256.degree., on shaking with a
 of NaOCl, finally at 65-70.degree., heating the reaction mixt. with solid
 KOH at 70-80.degree., extg. with ether and extg. the ether ext. with HCl;
 picrate, m. 210.degree. (decompn.). Ph2C(OH)CH2NH2.HCl, m. 191.degree.
 (decompn.), was prepd. from PhMgBr and glycine ester-HCl; picrate, m.
 179.degree. (decompn.). Ph2C(OH)CH(CH2Ph)NH2.HCl, m. 225-6.degree.
 (decompn.), was obtained by reaction of PhMgBr (from 35 g. PhBr) and 6 g.
 .beta.-phenylalanine ester-HCl in a yield of 4.5 g. The attempt to
 reduce dibenzyl ketoxime with Na-Hg to (PhCH2)2CHNH2 (III) was unsuccessful, due
 probably to strong steric hindrance. III was, however, prepd. by the
 modified Leuckart method (C. A. 30, 7550.3). (PhCH2)2CO (30 g.) and
 20-25 cc. HCONH2 were heated together at 175-85.degree. for 8 hrs. and worked
 up in the usual manner; III-HCl, m. 200-1.degree., yield 25 g.; III picrate,
 m. 191-2.degree.; N-formyl deriv. of III, m. 88-9.degree.. Condensation
 of 3.3 g. homopiperonylamine with crude Ph2CHCOCl (from 4.5 g. acid and
 excess SOCl2) in petr. ether yielded diphenylacetylhomopiperonylamide
 (IV), m. 139-40.degree., yield 2.6 g. IV (2.5 g.) on refluxing with 7
 cc. POCl3 and 20 cc. toluene gave 1-diphenylmethyl-3,4-dihydro-6,7-
 methylenedioxyisoquinoline (V), m. 125-6.degree., after sintering at
 120.degree.; yield 2.2 g. Crude V (2 g.) on heating with 10 g. Zn dust
 and 60 cc. H2SO4 (1:4) and evapn. of the reaction product in dil. HCl
 gave 1-diphenylmethyl-1,2,3,4-tetrahydro-6,7-methylenedioxyisoquinoline-HCl,
 m. 239.degree. (decompn.); yield 1.6 g.; N-Ac deriv., m. 172.degree.;
 picrate, m. 212-13.degree. (decompn.). I (2.4 g.) by condensation with
 o-O2NC6H4COCl in the usual way gave 4.6 g. crude o-
 nitrobenzoylhomoveratrylamine (VI), m. 142.degree. (purified product).
 VI

L4 ANSWER 47 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 compd. The above reactions do not permit, as yet, any definite
 conclusions as to the structure of the red product or the colorless
 crystals. It can only be stated that the cryst. compd. corresponds in
 compn. to about a mol. compd. of PhCH2NHLi and NH2Li. The red color may
 be ascribed to soln. of PhCH2NHLi in PhCH2NH2 with formation of a complex
 compd. The intense colors produced by some amines with even very dil.
 solns. of organo-Li compds. can be utilized for the detection of
 organically combined Li. The amine is merely added to the soln. in
 question, which is then titrated with an approx. N soln. of EtOH in ether
 to disappearance of the color. Of the amines thus far studied, PhCH2NH2
 and p-toluidine serve best as the indicator. The red of the PhCH2NH2
 soln. changes 2 drops before the end point to a yellow color which then
 disappears completely. With p-toluidine, on the other hand, the soln.
 gradually becomes deep violet during the titration and suddenly turns at
 the end point to a canary-yellow which persists on further addn. of alc.
 Preliminary expts. indicate the method is also applicable to K and Na but
 not to Mg compds.
 ACCESSION NUMBER: 1942:33168 CAPLUS
 DOCUMENT NUMBER: 36:33168
 ORIGINAL REFERENCE NO.: 36:5150h-1,5151a-1,5152a-h
 TITLE: A new reaction between benzylamine and alkali metals
 AUTHOR(S): Krabbe, Walter; Grunwald, Geza; Olzin, E.; Menzel, W.
 SOURCE: Ber. (1941), 74B, 1343-52
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 IT 57728-37-7, 1-Propanol, 2-amino-1,1,3-triphenyl-
 (reaction (color) with NaNH2)
 RN 57728-37-7 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl- (9CI) (CA INDEX
 NAME)



L4 ANSWER 48 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 (4.5 g.) on refluxing with 15 cc. POCl3 and 40 cc. toluene gave
 1-(o-nitrophenyl)-3,4-dihydro-6,7-dimethoxyisoquinoline (VII), m.
 117.degree. after slight shrinking at 112.degree.; yield 4.2 g. VII (1
 g.) yielded 1-(o-aminophenyl)-1,2,3,4-tetrahydro-6,7-
 dimethoxyisoquinoline, m. 162.degree., on heating with 10 g. Zn dust and
 60 cc. dil. H2SO4; hydrochloride, m. 189.degree. (decompn.) after
 sintering at 183.degree.; di-Ac deriv., m. 196.degree..
 ACCESSION NUMBER: 1942:10108 CAPLUS
 DOCUMENT NUMBER: 36:10108
 ORIGINAL REFERENCE NO.: 36:1603g-1,1604a-e
 TITLE: Synthetic experiments in the group of
 sympathomimetics. III
 AUTHOR(S): Rajagopalan, S.
 SOURCE: Proceedings - Indian Academy of Sciences, Section A
 (1941), 14A, 126-32
 CODEN: PISAA7; ISSN: 0370-0089
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 IT 23577-25-5, 1-Propanol, 2-amino-1,1,3-triphenyl-, -HCl
 (prepn. of)
 RN 23577-25-5 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, hydrochloride
 (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 49 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN

AB In the prepn. of tert. amino alcs. by means of the Grignard reagent either the free esters of amino acids or their HCl salts may be used. The latter give the better yields. The reaction was performed with the esters of glycine, alanine, PhCHNH₂CO₂H, phenylalanine, leucine and tyrosine and the Grignard reagent from PhBr, PhCH₂Br, EtBr and MeBr. The products contg. Ph and PhCH₂ were difficultly sol. in H₂O and sepd. out when NH₄OH was added to the acid soln. The Me and Et derivs. were sol. and could not be extd. satisfactorily with Et₂O; hence in the case of glycine and alanine the filtrate from the Mg(OH)₂ was benzoyleated and the Bz deriv. isolated. The amino alc. obtained from leucine and EtMgBr was insol. in 20% NaOH. 2-Amino-1,1-diphenyl-1-ethanol (I), m. 110-1.degree., was prepd. in 60% yield from CH₂NH₂CO₂Et and PhMgBr, and in 68% yield from the HCl salt. 2-Benzoylamino-1,1-diphenyl-1-ethanol (II), m. 182.degree., in 96% yield by benzylation of I. 2-Amino-1,1-diethyl-1-ethanol (III), m. 65-70.degree., in 24% yield from CH₂NH₂CO₂Et.HCl and EtMgBr and steam distn. of the product. 2-Benzoylamino-1,1-diethyl-1-ethanol (IV), m. 104.degree., in 58% yield from the crude HCl salt of III by treatment

with BzCl and NaOH. A yield of 62% was obtained from the free ester and Grignard reagent and benzylation of the reaction mixt. 2-Amino-1,1-dibenzyl-1-ethanol, m. 115-6.degree., in 49.2% yield from CH₂NH₂CO₂Et.HCl and PhCH₂MgBr. 2-Amino-1,1-diphenyl-1-propanol (V), m. 104-5.degree., in 59% yield from alanine ester and PhMgBr. HCl salt, m. 210-5.degree. (decompn.). V was obtained in 67% yield from the HCl salt of alanine ester. 2-Benzoylamino-1,1-diethyl-1-propanol (VI), m. 104-5.degree., in 52% yield by benzylation of the reaction mixt. from alanine ester and EtMgBr. From the ester-HCl the yield was 55%. 2-Amino-1,1,2-triphenyl-1-ethanol-HCl, m. 234-6.degree. (decompn.), from PhCHNH₂CO₂Et.HCl and PhMgBr. Free base (VII), m. 154.degree., yield 72%. 2-Amino-2-phenyl-1,1-diethyl-1-ethanol (VIII), m. 93-5.degree., in 65% yield from PhCHNH₂CO₂Et.HCl and EtMgBr. HCl salt, m. 214-5.degree.. 2-Benzoylamino-2-phenyl-1,1-diethyl-1-ethanol (IX), m. 173.degree., in

74% yield by benzylation of VIII. 2-Amino-2-phenyl-1,1-dibenzyl-1-ethanol, m. 125-6.degree. (yield 61%, from PhCHNH₂CO₂Et.HCl and PhCH₂MgBr. 2-Amino-1,1,3-triphenyl-1-propanol (X), m. 144-5.degree. (yield, 69%), from phenylalanine ester-HCl and PhMgBr. 3-Phenyl-2-amino-1,1-dibenzyl-1-propanol, m. 129-30.degree., in 58% yield from phenylalanine ester-HCl and PhCH₂MgBr. 3-Phenyl-2-amino-1,1-diethyl-1-propanol (XI), oil b16-7 145-8.degree., from the same and EtMgBr. 3-Phenyl-2-benzoylamino-1,1-diethyl-1-propanol, m. 135.degree., by benzylation of XI.

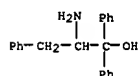
ACCESSION NUMBER: 1925:4548 CAPLUS
DOCUMENT NUMBER: 19:4548
ORIGINAL REFERENCE NO.: 19:635e-1, 636a
TITLE: The action of the Grignard reagent on amino acids. I
AUTHOR(S): Thomas, Karl; Bettzieche, Fritz
SOURCE: Z. physiol. Chem. (1924), 140, 244-60
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 57728-37-7, 1-Propanol, 2-amino-1,1,3-triphenyl- (prepn. of)
RN 57728-37-7 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha., .alpha.-diphenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 50 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN

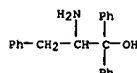
AB To det. whether aromatic amides RCONHC₆H₄R', in the same manner as aryl sec. amines, substitute H of the NH group by treatment with alcs., PhNHAc (A) was dissolved in a large excess of warm MeOH, and the soln. in vapor form directed against Al₂O₃ heated to 370-80.degree.; continuous formation of Me₂O took place, and a liquid product condensed which sepd. at once into 2 layers, one being H₂O and unchanged MeOH with a little Me₂O, the second a yellow oil b. 187-200.degree., consisting of PhNH₂ (B), PhNHMe, and PhNHMe₂; a residue of unchanged A remained; no exalgine (PhNHMeAc) was found: H₂O from MeOH hydrolyzed A, the resulting B being then methylated. A with EtOH or with PrOH reacts in a way entirely parallel to the above; in addn., traces resp. of AcH, and of MeAcH and CH₃CH:CH₂, are formed,

but no PhNR₂. Propionanilide, isovalerianilide, o-acetotoluide, and o-benzotoluide all react like A. It appears impossible to alkylate the NH group of aromatic amides by this catalysis.

ACCESSION NUMBER: 1923:8132 CAPLUS
DOCUMENT NUMBER: 17:8132
ORIGINAL REFERENCE NO.: 17:1439a-c
TITLE: The action of alcohols on anilides
AUTHOR(S): Mailhe, Alphonse
SOURCE: Bull. soc. chim. (1923), 33, 81-3
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 57728-37-7, 1-Propanol, 2-amino-1,1,3-triphenyl- (prepn. of)
RN 57728-37-7 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha., .alpha.-diphenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 49 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)

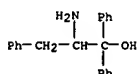


L4 ANSWER 51 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN

AB H₂NCHPhCPh₂OH was prepd. by the action of an excess of PhMgBr upon H₂NCHPhCO₂H or the Et ester. The reaction product from MeMgI would not cryst. and that from .alpha.-ClO₇MgBr contained no N and formed lustrous plates, m. 65.5-6.5.degree.. The action of HNO₂ upon H₂NCHPhCPh₂OH invariably gave HOCPh:CPh₂ in about 70% yield. The action of HNO₂ upon H₂NCHPhCPhMeOH gave CHMePhCOPh, prisms, m. 59.5-6.degree. (Meyer, Ber.

21, 1297, gives 53.degree.). Semicarbazone, prismatic needles, m. 161.degree.. H₂NCHPhCPh(C10H₇)OH gave either naphthyldeoxybenzoin or one of its desmotropic isomers, forming rectangular prisms, m. 107-8.degree.. .gamma.-Hydroxy-.alpha., .gamma., .gamma.-triphenylpropylamine, prismatic needles, m. 146.5-7.5.degree., and gives a reddish orange color with concd. H₂SO₄. HNO₂ gives HOCHPhCH₂CPh₂OH. Ethylphenylalanine hydrochloride, needles, m. 124-5.degree.. With PhMgBr this yields .gamma.-hydroxy-.alpha., .gamma., .gamma.-triphenylisopropylamine, glassy needles, m. 144.5-5.5.degree.. HNO₂ gives a compound (probably diphenylmethyl benzyl ketone), rosos of glassy needles, m. 121.5-2.degree.. Reactions with other tert. NH₂ alcs. are reviewed.

ACCESSION NUMBER: 1923:8131 CAPLUS
DOCUMENT NUMBER: 17:8131
ORIGINAL REFERENCE NO.: 17:1438g-1, 1439a
TITLE: Elimination of the amino group in tertiary amino alcohols. I
AUTHOR(S): McKenzie, Alex.; Richardson, A. C.
SOURCE: Journal of the Chemical Society, Abstracts (1923), 123, 79-81
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 57728-37-7, 1-Propanol, 2-amino-1,1,3-triphenyl- (prepn. of)
RN 57728-37-7 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha., .alpha.-diphenyl- (9CI) (CA INDEX NAME)



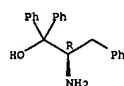
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L4 ANSWER 1 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN
 AB The compds. are prepd. by reaction of amino acids with RMgCl [R = (un)substituted aliph. group, arom. group], acid-treated with aq. H2SO4 soln., and alkali-treated with NH3. 2-Chloroanisole was reacted Mg in the presence of dibromoethane in THF-PhMe at 85.degree. for 10 h, mixed with D-alanine Et ester hydrochloride at 25.degree. for 2.5 h, and treated with aq. H2SO4 soln. and aq. NH3 soln. to give 82.6% (R)-2-amino-1,1-di-(2-methoxyphenyl)propanol.

ACCESSION NUMBER: 2003:257865 CAPLUS
 DOCUMENT NUMBER: 138:271376
 TITLE: Preparation of amino alcohols
 INVENTOR(S): Hirota, Masashi; Itagaki, Makoto; Hagitani, Hirotochi
 PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKKXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003096036	AZ	20030403	JP 2001-290834	20010925
PRIORITY APPLN. INFO.: JP 2001-290834 20010925				
OTHER SOURCE(S): CASREACT 138:271376; MARPAT 138:271376				
IT 86906-05-0P				
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)				
(prepn. of amino alcs. by reaction of amino acids with Grignard reagents and treatment with H2SO4 and NH3)				
RN	86906-05-0 CAPLUS			
CN	Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.R)- (9CI) (CA INDEX NAME)			

Absolute stereochemistry.

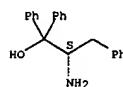


L4 ANSWER 2 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L4 ANSWER 2 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN
 AB .beta.-Amino alcs. were easily prepd. from L-phenylalanine in three simple straightforward steps. The key intermediate compd. (-)-(.alpha.S)-.alpha.- (phenylmethyl)-1-piperidineacetic acid Me ester was achieved in high yield (up to 92%) with glutaraldehyde and NaBH4/H2SO4 in THF at room temp. Amino alcs. thus prepd. included (.beta.S)-.alpha.,.alpha.-diphenyl-.beta.- (phenylmethyl)-1-piperidineethanol, (.beta.S)-.alpha.,.alpha.-dimethyl-.beta.- (phenylmethyl)-1-piperidineethanol, (.beta.S)-.alpha.,.alpha.-diethyl-.beta.- (phenylmethyl)-1-piperidineethanol (I), and (.beta.S)-.alpha.,.alpha.-dipropyl-.beta.- (phenylmethyl)-1-piperidineethanol (II), and (-)-1-[(1S)-2-phenyl-1-(1-piperidinyl)ethyl]cyclopentanol. These five ligands were applied to catalyze enantioselective addn. of di-Et zinc to aldehydes, high asym. induction was obsd. with I and II, and the ee value was up to 98%. The effect of the substituents on the nitrogen atom was also obsd. via comparing piperidine-based amino alcs. with pyrrolidine-based similar ligands. (.beta.S)-.alpha.,.alpha.-Diethyl-.beta.- (phenylmethyl)-1-Pyrrolidineethanol and (.beta.S)-.alpha.,.alpha.-diphenyl-.beta.- (phenylmethyl)-1-Pyrrolidineethanol were less efficient ligands.

ACCESSION NUMBER: 2003:149318 CAPLUS
 DOCUMENT NUMBER: 139:149370
 TITLE: A convenient synthesis of piperidine-based .beta.-amino alcohols from l-Phe and highly enantioselective addition of diethyl zinc to aldehydes
 AUTHOR(S): Da, Chao-shan; Han, Zhi-jian; Ni, Ming; Yang, Fan; Liu, Da-xue; Zhou, Yi-feng; Wang, Rui
 CORPORATE SOURCE: School of Life Sciences, Department of Biochemistry & Molecular Biology, Lanzhou University, Lanzhou, 730000, Peop. Rep. China
 SOURCE: Tetrahedron: Asymmetry (2003), 14(6), 659-665
 CODEN: TASYE3; ISSN: 0957-4166
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 IT 79868-78-3P, (.beta.S)-.beta.-Amino-.alpha.,.alpha.-diphenylbenzenepropanol
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of piperidine-based .beta.-amino alcs. from L-phenylalanine and highly enantioselective addn. of di-Et zinc to aldehydes)
 RN 79868-78-3 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

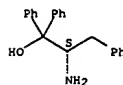


REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 3 OF 51 CAPLUS COPYRIGHT 2003 ACS ON STN
 AB A general methodol. has been evaluated for the prepn. and optimization and fine-tuning of polymer-supported chiral catalysts for the ZnEt2 addn. to benzaldehyde. This approach involves the use of parallel solid-phase chem. and the use of cheap and easily available chiral starting materials, such as amino acids. In this way, small, focused polymer-supported libraries of .alpha.,.alpha.-substituted amino alcs. have been prepd. and evaluated as chiral ligands for the above-mentioned catalytic reaction. This strategy allows for an easy and fast way to analyze the different factors affecting the efficiency of the supported species (including the polymeric network itself) and to improve the tuning of the chiral catalysts. For the cases studied, amino alcs. contg. aliph. .alpha.-substituents have been shown to give good results when in conjunction with both aliph. side chains at the .beta. position and a N-Me substituent.

ACCESSION NUMBER: 2003:128975 CAPLUS
 DOCUMENT NUMBER: 139:52712
 TITLE: Development of small focused libraries of supported amino alcohols as an efficient strategy for the optimization of enantioselective heterogeneous catalysts for the ZnEt2 addition to benzaldehyde
 AUTHOR(S): Isabel Burguete, M.; Collado, Manuel; Garcia-Verdugo, Eduardo; Vicent, Maria J.; Luis, Santiago V.; Graf von Keyserling, Nikolai; Martens, Jurgen
 CORPORATE SOURCE: E.S.T.C.E., Departamento de Quimica Inorganica y Organica, Universitat Jaume I, Castellon, E-12080, Spain
 SOURCE: Tetrahedron (2003), 59(10), 1797-1804
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 IT 79868-78-3DP, polymer-supported
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (enantioselective addn. of diethylzinc to benzaldehyde catalyzed by polymer-supported chiral amino alcs.)
 RN 79868-78-3 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

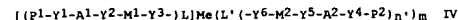
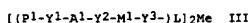
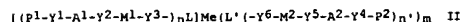
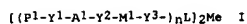


REFERENCE COUNT: 96 THERE ARE 96 CITED REFERENCES AVAILABLE FOR THIS

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FORMAT

L4 ANSWER 4 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
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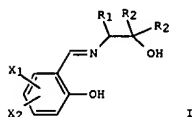
AB The present invention involves the use of chiral, uncharged compds. as doping agents for liq. crystals. The indicated compds. are I or II, for which the variables are defined, independently of each other, as follows:
or P1 and P2 are H, C1-C12 alkyl groups, a polymerizable or polymd. group,

a group contg. such a polymerizable group; Y1 through Y6 are groups -O-, -S-, -CO-, -CO-O-, -O-CO-, -CO-N(R)-, -(R)N-CO-, -O-CO-O-, -O-CO-N(R)-, (R)N-CO-O-, or -(R)N-CO-N(R)-; R is H or a C1-C4 alkyl; A1 and A2 are spacers with up to 30 C atoms; M1 and M2 are mesogen groups; n' and n equal 0 or 1; m is 1, 2, or 3, in which the group L'(-Y6-M2-Y5-A2-Y4-P2)n in formula II can represent different moieties; Me is either a transition metal of the 4th, 5th, or 6th period (with the exception of Tc, Ag, Cd, Au, Hg, and the lanthanides) or a Group IVA element (with the exception of C and Pb); L is a tridentate ligand including N-, O-, P-, or S-contg. groups, over which .gtoreq.1 free electron pair is available for coordination to the metal Me; and L' is an org. group with up to 12 C atoms. The invention also includes compds. III and IV, for which all variables are the same as for the previous compd., as well as liq. cryst. compds. contg. .gtoreq.1 of the indicated compds.

ACCESSION NUMBER: 2002:446122 CAPLUS
DOCUMENT NUMBER: 137:26396
TITLE: Use of chiral, uncharged metal compounds as doping agents for liquid crystals
INVENTOR(S): Prechtel, Frank; Haremza, Sylke; Parker, Robert; Kuerschner, Kathrin; Braun, Manfred; Hahn, Antje; Fleischer, Ralf
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: Eur. Pat. Appl., 26 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1213293	A1	20020612	EP 2001-128679	20011201
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

L4 ANSWER 5 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
GI



AB Chiral copper complex catalyst compns. obtained by contacting an optically active N-salicylideneaminoalc. compd. (I) with a monovalent or divalent copper compd. in an inert solvent, where R1 and R2 represent an alkyl group and the like, X1 and X2 represent a hydrogen atom, a halogen atom, a nitro group, an alkyl group, an alkoxy group, a cyano group or the like, and the amt. of the monovalent or divalent copper compd. is <1 mol per mol of I. A process for producing an optically active cyclopropane-carboxylic acid ester using the chiral copper catalysts is described. Thus, (R)-N-salicylidene-2-amino-1,1-di(2-butoxy-5-tert-butylphenyl)-1-propanol was prepd. and mixed with copper naphthenate or copper acetate monohydrate in toluene to generate an optically active copper complex catalyst soln. Cis and trans-chrysanthemic acid Et ester were prepd. (.apprxq.60:40 trans:cis) with enantiomeric excesses of up to 71% for the trans isomer and 60% for the cis isomer were prepd. using the chiral copper catalyst compna.

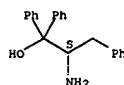
ACCESSION NUMBER: 2001:559583 CAPLUS
DOCUMENT NUMBER: 135:137235
TITLE: Chiral copper complex catalyst compositions for use in asymmetric production process of cyclopropanecarboxylic acid esters
INVENTOR(S): Suzuki, Gohfu; Itagaki, Makoto; Yamamoto, Michio
PATENT ASSIGNEE(S): Sumitomo Chemical Company, Limited, Japan
SOURCE: Eur. Pat. Appl., 22 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1120401	A2	20010801	EP 2001-101450	20010123
EP 1120401	A3	20020123		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 2001037036	A1	20011101	US 2001-766579	20010123
US 6469198	B2	20010122		
CN 1314209	A	20010926	CN 2001-111976	20010125
JP 2001278851	A2	20011010	JP 2001-16782	20010125
PRIORITY APPLN. INFO.:			JP 2000-16279	A 20000125

L4 ANSWER 4 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

DE 10061625 A1 20020613 DE 2000-10061625 20001211
JP 2002220366 A2 20020809 JP 2001-377549 20011211
US 2003066984 A1 20030410 US 2001-11748 20011211
PRIORITY APPLN. INFO.: DE 2000-10061625 A 20001211
IT 79868-78-3P, (2S)-2-Amino-2-benzyl-1,1-diphenylethanol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(use of chiral, uncharged metal compds. as doping agents for liq. crystals)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



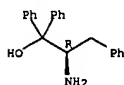
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 5 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

OTHER SOURCE(S): MARPAT 135:137235
IT 86906-05-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for prepn. of chiral copper(I) and copper(II) salicylideneaminoalc. complex catalyst compns. for use in asym. synthesis of cyclopropanecarboxylic acid esters)
RN 86906-05-0 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



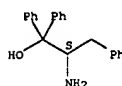
L4 ANSWER 6 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB The use of 10 mol% racemic amino alc. Me3CCH(OH)NR1 [1, NR1 = piperidino, 2,6-dimethylpiperidino, morpholino, pyrrolidino, dicyclohexylamino] and 5 mol% of a chiral amino acid-derived amino alc. gave chiral induction in the ethylation of arom. aldehydes with Et2Zn. The best combinations were 1 [NR1 = piperidino, 2,6-dimethylpiperidino] and (S)-HOCPh2CH(NH2)CH2Ph or (S)-.alpha.,.alpha.-diphenylpyrrolidinemethanol. The chiral amino alc. is postulated to work by deactivating one isomer of the intermediate Zn complex.

ACCESSION NUMBER: 2001:140895 CAPLUS
 DOCUMENT NUMBER: 134:340317
 TITLE: Engineering catalysts for enantioselective addition of diethylzinc to aldehydes with racemic amino alcohols: nonlinear effects in asymmetric deactivation of racemic catalysts

AUTHOR(S): Long, Jiang; Ding, Kuiling
 CORPORATE SOURCE: Laboratory of Organometallic Chemistry Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
 SOURCE: Angewandte Chemie, International Edition (2001), 40(3), 544-547
 CODEN: ACIEF5; ISSN: 1433-7851
 PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:340317
 IT 79868-78-3
 RL: CAT (Catalyst use); USES (Uses)
 (enantioselective addn. of diethylzinc to aldehydes catalyzed by a mixt. of racemic and chiral amino alcs.)

RN 79868-78-3 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
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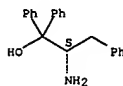
L4 ANSWER 7 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB Resin-supported chiral amino alcs. bound to polymeric network via a sulfonamide link are prepd. very efficiently from polymeric N-tosyl amides of amino acid esters. Preliminary results from stereoselective redn. of PhAc show that those compds. can be used as chiral auxiliaries. The presence of the sulfonyl group plays an important role in detg. the properties of the resulting supported reagents.

ACCESSION NUMBER: 2001:128874 CAPLUS
 DOCUMENT NUMBER: 134:325996
 TITLE: A general route for the preparation of polymer-supported N-tosyl amino alcohols and their use as chiral auxiliaries

AUTHOR(S): Altava, B.; Burguete, M. I.; Collado, M.; Garcia-Verdugo, E.; Luis, S. V.; Salvador, R. V.; Vicent, M. J.
 CORPORATE SOURCE: ESTCE, Department of Inorganic and Organic Chemistry, University Jaume I, Castellon, Spain
 SOURCE: Tetrahedron Letters (2001), 42(9), 1673-1675
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:325996
 IT 79868-78-3D, resin-bound
 RL: CAT (Catalyst use); RGT (Reagent); RACT (Reactant or reagent); USES (Uses)
 (polymer-supported N-tosyl amino alcs. as chiral auxiliaries for asym. redn.)

RN 79868-78-3 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS
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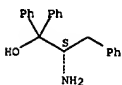
L4 ANSWER 8 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB The title compds., 2-[(pyridinyl)methyl]amino ethanol derivs., were conveniently prepd. from .beta.-amino alcs. through a two-step reaction and applied to catalyze the enantioselective addn. of diethylzinc to benzaldehyde. Among them, (-)-.alpha.-[(1S)-2-methyl-1-[[2-(pyridinyl)methyl]amino]propyl]-.alpha.-phenylbenzenemethanol was found to show the best asym. induction and catalyze the reaction of various arom. aldehydes to provide (R)-secondary alcs. in up to 98.3% ee.

ACCESSION NUMBER: 2000:845060 CAPLUS
 DOCUMENT NUMBER: 134:115544
 TITLE: Synthesis of N-.alpha.-pyridylmethyl amino alcohols and application in catalytic asymmetric addition of diethylzinc to aromatic aldehydes

AUTHOR(S): Wu, Yangjie; Yun, Hongying; Wu, Yusheng; Ding, Kuiling; Zhou, Ying
 CORPORATE SOURCE: Department of Chemistry, Zhengzhou University, Zhengzhou, 450052, Peop. Rep. China
 SOURCE: Tetrahedron: Asymmetry (2000), 11(17), 3543-3552
 CODEN: TASYE3; ISSN: 0957-4166
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:115544
 IT 79868-78-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of [(pyridinyl)methyl]amino ethanol derivs. as ligands for asym. addn. of diethylzinc to arom. aldehydes)

RN 79868-78-3 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS
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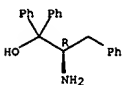
L4 ANSWER 9 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB Modified guanidines were explored as potential chiral superbases. Thus, chiral 1,3-dimethyl-2-iminoimidazolidines with or without 4,5-di-Ph groups, their guanidinium salts, and the 2-iminoimidazolidines with (S)-1-phenylethyl groups on the ring nitrogens were prepd. by treatment of 2-chloroimidazolidinium chlorides with appropriate amines. Bicyclic guanidines were also prepd. from a prolinamide using a similar procedure.

ACCESSION NUMBER: 2000:742505 CAPLUS
 DOCUMENT NUMBER: 134:56616
 TITLE: Modified Guanidines as Potential Chiral Superbases. 1. Preparation of 1,3-Disubstituted and the Related Guanidines through Chloroamidine Derivatives

AUTHOR(S): Isobe, Toshio; Fukuda, Keiko; Ishikawa, Tutomu
 CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Chiba University, Inage Chiba, 263-8522, Japan
 SOURCE: Journal of Organic Chemistry (2000), 65(23), 7770-7773
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:56616
 IT 86906-05-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of 1,3-disubstituted 2-iminoimidazolidines and the related guanidines)

RN 86906-05-0 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.R)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
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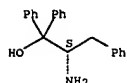
L4 ANSWER 10 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 AB The of enantioselective redn. 1-bromofluorenone by borane in the presence of different chiral amino alcs. has been studied. The alc. obtained has the (S) or (R) configuration depending on the nature of the substitution of the amino alc. The exptl. detd. abs. configuration can be explained when a four-center cyclic transition state consisting of the oxazaborolidine and fluorenone compd. is considered.

ACCESSION NUMBER: 2000:656730 CAPLUS
 DOCUMENT NUMBER: 134:4737
 TITLE: Study of asymmetric reduction of 1-substituted fluorenone with borane in the presence of several chiral amino alcohols

AUTHOR(S): Yu, Z.; Lopez-Calahorra, F.; Velasco, D.
 CORPORATE SOURCE: Facultat de Química, Departamento de Química Organica,
 SOURCE: Universitat de Barcelona, Barcelona, E-08028, Spain
 PUBLISHER: Tetrahedron: Asymmetry (2000), 11(15), 3221-3225
 DOCUMENT TYPE: CODEN: TASYE3; ISSN: 0957-4166
 LANGUAGE: Elsevier Science Ltd.
 OTHER SOURCE(S): Journal
 IT 79868-78-3 English
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asym. redn. of 1-bromofluorenone with borane in the presence of chiral amino alcs.)

RN 79868-78-3 CAPLUS
 CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
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L4 ANSWER 11 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
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AB Title compds. [I: R = C(R2)3; R2 = H, (un)substituted alk(en)yl, etc.; R4 = e.g., NH2; R5 = C(R3)2R6; R3 = H, halo, alkyl, aryl, etc.; R6 = H or halo] were prepd. by treating I [R4R5 = e.g., NHCO2C(R3)2] with H or an H halide. Thus, (S)-Me2CHCH(NH2)CO2Me was treated with excess PhMgBr and the product cyclocondensed with ClCO2CCl3 to give (S)-I (R = Me2, R4R5 = NHCO2CPh2) which was treated with H/Pd to give (S)-Me2CHCH(NH2)CHPh2.

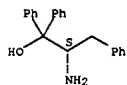
ACCESSION NUMBER: 2000:401763 CAPLUS
 DOCUMENT NUMBER: 133:43300
 TITLE: Preparation of .alpha.,.alpha.-diarylalkanamine and analog enantiomers

INVENTOR(S): O'Hagan, David
 PATENT ASSIGNEE(S): University of Durham, UK
 SOURCE: PCT Int. Appl., 48 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034210	A1	20000615	WO 1999-GB4031	19991206
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TH				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, NG, TD, TG				
EP 1135349	A1	20010926	EP 1999-959517	19991206
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRIORITY APPLN. INFO.: GB 1998-26700 A 19981205 WO 1999-GB4031 W 19991206				
OTHER SOURCE(S): CASREACT 133:43300; MARPAT 133:43300				
IT 79868-78-3P RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of .alpha.,.alpha.-diarylalkanamine and analog enantiomers)				
RN 79868-78-3 CAPLUS				
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)				

Absolute stereochemistry. Rotation (-).

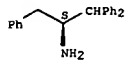
L4 ANSWER 11 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



IT 233772-38-8P
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of .alpha.,.alpha.-diarylalkanamine and analog enantiomers)

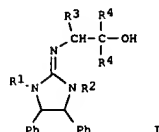
RN 233772-38-8 CAPLUS
 CN Benzenepropanol, .beta.-phenyl-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L4 ANSWER 12 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
 GI



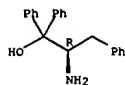
AB Title compds. I (R1, R2 = alkyl; R3 = alkyl, aryl, aralkyl; R4 = H, aryl), useful as reagents for asym. reaction, are prepd. (4S,5S)-2-chloro-4,5-diphenyl-1,3-dimethylimidazolidinium chloride was reacted with (R)-phenylalaninol in CH2Cl2 in the presence of Et3N at room temp. for 30 min to give 85% (4S,5S)-4,5-diphenyl-2-((1R)-1-benzyl-2-hydroxyethyl)imino-1,3-dimethylimidazolidine (II). Dibenzyl 3-oxocyclopentylmalonate was prepd. with R:S ratio of 75.5:24.5 by reaction of 2-cyclopentenone with dibenzyl malonate in the presence of II.

ACCESSION NUMBER: 1999:680124 CAPLUS
 DOCUMENT NUMBER: 131:286519
 TITLE: Preparation of optically active 4,5-diphenyl-1,3-dialkyl-2-(2-hydroxyethyl)iminoimidazolidines

INVENTOR(S): Isobe, Toshio; Fukuda, Keiko
 PATENT ASSIGNEE(S): Shiratori Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKOXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11292850	A2	19991026	JP 1998-97208	19980409
PRIORITY APPLN. INFO.: JP 1998-97208 19980409				
OTHER SOURCE(S): MARPAT 131:286519				
IT 86906-05-0 RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. of optically active diphenyldialkyl(hydroxyethyl)iminoimidazolidines as reagents for asym. reaction)				
RN 86906-05-0 CAPLUS				
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.R)- (9CI) (CA INDEX NAME)				

Absolute stereochemistry.



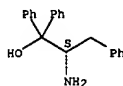
AB Starting from simple amino acid esters and Merrifield resins, a small library of polymer-bound chiral-.beta.-amino alcs. is prepd. By reaction with LiAlH₄, the corresponding chiral reducing agents are obtained, having structural variations at both the .alpha. and .beta. positions. All supported reagents are able to reduce PhAc to PhCHMeOH. Enantioselectivity is obsd. when the steric hindrance in the chiral fragment is increased. Best results are obtained for the supported deriv. of .alpha.,.alpha.-diphenyl-phenylalaninol.

ACCESSION NUMBER: 1999:559559 CAPLUS
DOCUMENT NUMBER: 131:257843
TITLE: Small libraries of polymer-supported amino alcohols. An application to the enantioselective reduction of acetophenone by LAH

AUTHOR(S): Altava, B.; Burgette, M. I.; Garcia-Verdugo, E.; Luis, S. V.; Pozo, O.; Salvador, Rosa V.
CORPORATE SOURCE: Dep. Quimica Inorganica Organica, E.S.T.C.E., Univ. Jaume I, Castellon, E-12080, Spain
SOURCE: European Journal of Organic Chemistry (1999), (9), 2263-2267
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:257843
IT 79868-78-3DP, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of libraries of polymer-supported amino alcs. as catalysts for asym. redn. of acetophenone by LiAlH₄)

RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

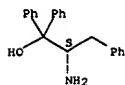
AB New, chiral .beta.-tert-amino tert-alcs. were synthesized from an enantiomerically pure sec-amine via glycine, alanine and phenylglycine derivs. Grignard addns. to these esters provided rigid amino alcs. in fair yields. The abs. configurations of the stereogenic centers, which arose during the alkylation step, were assigned by an independent route leading to some of the optical antipodes. The target compds. were derivs. of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol. Condensation of enantiomerically pure .beta.-amino alcs. with a .gamma.-keto ester afforded N,O-acetals which were subsequently reduced to the .beta.-tert-amino alcs. X-Ray anal. of one compd. was performed to verify the stereochem. obsd. by chem. correlation. The nucleophilic ring opening of enantiomerically pure styrene oxide by an amine resulted in the formation of regioisomeric amino alcs. Amino thiol derivs. were also prepd. Redn. of these compds. to thiols and subsequent oxidn. afforded amino disulfides. Finally, the bicyclic .beta.-amino alcs. and thiols were used as chiral ligands in the enantioselective addn. of diethylzinc to benzaldehyde and ee values up to 96% were found.

ACCESSION NUMBER: 1999:497835 CAPLUS
DOCUMENT NUMBER: 131:350834
TITLE: Utilization of industrial waste materials. Part 14. Synthesis of .beta.-amino alcohols and thiols with a 2-azabicyclo[3.3.0]octane backbone and their application in enantioselective catalysis

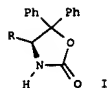
AUTHOR(S): Kossenjans, Michael; Soeberdt, Michael; Wallbaum, Sabine; Harms, Klaus; Martens, Jürgen; Aurich, Hans Günter
CORPORATE SOURCE: Fachbereich Chemie, Universität Oldenburg, Oldenburg, D-26129, Germany
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (16), 2253-2365
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:350834
IT 79868-78-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addn. catalysts)

RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



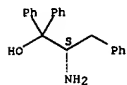
REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT



AB A range of (S)-.alpha.-(diphenylmethyl)alkyl amines RCH(NH₂)CHPh₂ (R = CHMe₂, CH₂Ph, Me, CHMeEt, CH₂CHMe₂) were prepd. from the corresponding (S)-.alpha.-amino acid ester hydrochlorides. These amines were derived

by direct hydrogenation of their precursor oxazolidinones I.
ACCESSION NUMBER: 1999:327837 CAPLUS
DOCUMENT NUMBER: 131:129717
TITLE: A short synthesis of (S)-.alpha.-(diphenylmethyl)alkyl amines from amino acids
AUTHOR(S): O'Hagan, David; Tavasli, Mustafa
CORPORATE SOURCE: Department of Chemistry, Science Laboratories, University of Durham, Durham, DH1 3LE, UK
SOURCE: Tetrahedron: Asymmetry (1999), 10(6), 1189-1192
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:129717
IT 79868-78-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of (diphenylmethyl)alkyl amines from amino acids)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



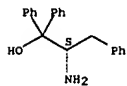
IT 233772-38-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of (diphenylmethyl)alkyl amines from amino acids)
RN 233772-38-8 CAPLUS
CN Benzenethanamine, .beta.-phenyl-.alpha.-(phenylmethyl)-, (.alpha.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

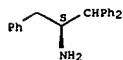
AB A new design of cryst. hosts derived from amino acids, characterized by an aminoethanol functional unit or its carbonamide structural deriv. and appended arom. residues including secondary substituents, is reported. Fifteen host compds., including (S)-2-amino-1,1-bis(4-tert-butylphenyl)-1-propanol (3) and (S)-2-(dibenzylamino)-1,1-diphenyl-1-propanol (11), were synthesized. Cryst. inclusion formation is shown and discussed with ref. to structural parameters of the host mols. X-Ray crystal structures of compds. 3 and 11 have been detd. in order to suggest reasons for their failure to show inclusion ability.

ACCESSION NUMBER: 1999:210874 CAPLUS
DOCUMENT NUMBER: 130:352509
TITLE: Supramolecular inclusion hosts based on amino acid compound sources: design, synthesis and crystalline inclusion behavior. X-ray crystal structures of two inefficient host compounds
AUTHOR(S): Weber, Edwin; Reutel, Christiane; Foces-Foces, Concepcion; Llamas-Saiz, Antonio L.
CORPORATE SOURCE: Institut für Organische Chemie der Technischen Universität Bergakademie Freiberg, Freiberg/Sachsen, D-09596, Germany
SOURCE: Journal of Inclusion Phenomena and Macrocyclic Chemistry (1999), 33(1), 47-68
CODEN: JIPCF5
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 79868-78-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of supramol. inclusion hosts based on amino acids and crystal structures of two inefficient host compds.)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

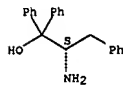


IT 224639-31-0P 224639-37-6P 224639-43-4P
224641-08-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of supramol. inclusion hosts based on amino acids and crystal structures of two inefficient host compds.)
RN 224639-31-0 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)-, compd. with 1-propanamine (3:1) (9CI) (CA INDEX NAME)
CM 1
CRN 79868-78-3
CMF C21 H21 N O



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

Absolute stereochemistry. Rotation (-).

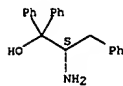


CM 2
CRN 107-10-8
CMF C3 H9 N

H₃C-CH₂-CH₂-NH₂

RN 224639-37-6 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)-, compd. with piperidine (2:3) (9CI) (CA INDEX NAME)
CM 1
CRN 79868-78-3
CMF C21 H21 N O

Absolute stereochemistry. Rotation (-).

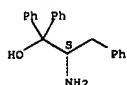


CM 2
CRN 110-89-4
CMF C5 H11 N



RN 224639-43-4 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)-, compd. with tetrahydrofuran (1:1) (9CI) (CA INDEX NAME)
CM 1
CRN 79868-78-3

Absolute stereochemistry. Rotation (-).



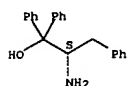
CM 2
CRN 109-99-9
CMF C4 H8 O



RN 224641-08-1 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha...alpha.-diphenyl-, (.beta.S)-, compd. with cyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1
CRN 79868-78-3
CMF C21 H21 N O

Absolute stereochemistry. Rotation (-).



CM 2
CRN 108-91-8
CMF C6 H13 N



REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 17 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
AB 4-Isopropyl-5,5-diphenyloxazolidinone (I) is readily prepd. from (R)- or (S)-valine ester, PhMgBr, and ClCO2Et. It has a m.p. of .apprx.250.degree., a low soly. in most org. solvents, and a C=O group which is sterically protected from nucleophilic attack. Thus, sol. N-acyloxazolidinones are prepd. from I with BuLi at temps. around 0.degree. instead of -78.degree., their Li.enolates can be generated with BuLi, rather than with LDA, and deacylation in the final step of the procedure can be achieved with NaOH at ambient temps., with facile recovery of the pptg. auxiliary I (filtering, washing, and drying). Alkylations, aminomethylations and hydroxymethylations, aldol addns., Michael addns., and a (4+2) cycloaddn. of N-acyloxazolidinones from I

were investigated. The well-known features of reactions following the Evans methodol. (yield, diastereoselectivity, dependence on conditions, counter ions, additives etc.) prevail in these transformations. Most products, however, have higher m.p.s. and a much more pronounced crystn. tendency than those derived from conventional oxazolidinones, and can thus be purified by recrystn., avoiding chromatog. The disadvantage of I having

a higher mol. wt. (.apprx.150 Da) than the non-phenyl-substituted auxiliary is more than compensated by the ease of its application, esp. on large scale. A no. of crystal structures of oxazolidinones derived from I and

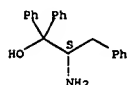
a TiCl4 complex of an oxazolidinone are described and discussed in view of the diastereoselective reaction mechanisms.

ACCESSION NUMBER: 1998:756309 CAPLUS
DOCUMENT NUMBER: 130:81445
TITLE: A useful modification of the Evans auxiliary.
4-Isopropyl-5,5-diphenyloxazolidin-2-one
AUTHOR(S): Hintermann, Tobias; Seebach, Dieter
CORPORATE SOURCE: Laboratorium Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Switz.
SOURCE: Helvetica Chimica Acta (1998), 81(11), 2093-2126
PUBLISHER: CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Verlag Helvetica Chimica Acta AG
LANGUAGE: Journal
OTHER SOURCE(S): English
IT 79868-78-3P CASREACT 130:81445

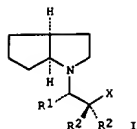
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and utilization of isopropylphenyloxazolidinone as chiral auxiliary)

RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha...alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



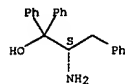
REFERENCE COUNT: 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT



AB Enantipure azabicyclooctane I (R1 = Me, CHMe2, CH2Ph, R2 = H; R1 = CH2Ph, Me, Ph, R2 = Ph; R1 = Ph, R2 = H, X = OH) were prepd. by condensation of .beta.-amino alcs. H2NCH(R1)R2 with Et (2-oxocyclopentyl)acetate and subsequent reductn. of the intermediate 9-oxa-1-azabicyclo[6.3.0.0.4,8]undecan-2-ones. I (R1 = Me, R2 = H, X = OH) was converted to I (X = SH) via I (X = SCOMe). With compds. I as chiral ligands in the reaction of benzaldehyde with diethylzinc, an enantiomeric excess between 14 and 84% was achieved.

ACCESSION NUMBER: 1998:257581 CAPLUS
DOCUMENT NUMBER: 128:308370
TITLE: Functionalized 2-azabicyclo[3.3.0]octanes as ligands in the enantioselective catalysis
AUTHOR(S): Aurich, Hans Gunter; Soeberdt, Michael
CORPORATE SOURCE: Fachbereich Chemie, Philipps-Universität Marburg, Marburg, D-35032, Germany
SOURCE: Tetrahedron Letters (1998), 39(17), 2553-2554
CODEN: TETLEA; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 79868-78-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of azabicyclooctanes as ligands for enantioselective addn. of benzaldehyde to diethylzinc)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

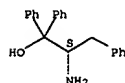


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

AB A general methodol. has been evaluated for the prepn. of polystyrene-divinylbenzene resins which contain chiral groups derived from simple amino acids. This approach requires the initial anchoring of an amino acid Me ester followed by the modification of the resulting polymers using solid-phase techniques. The appropriate transformations of the supported chiral groups can be accomplished very efficiently. Results obtained are much better than those described for similar reactions carried out in soln.

ACCESSION NUMBER: 1997:729068 CAPLUS
DOCUMENT NUMBER: 127:359062
TITLE: Preparation of polystyrene resins containing chiral groups derived from amino acids
AUTHOR(S): Altava, Belen; Burguete, M. Isabel; Collado, Manuel; Luis, Santiago V.; Poro, Oscar; Salvador, Rosa V.
CORPORATE SOURCE: Departamento de Química Inorgánica y Orgánica, ESTCE, Universitat Jaume I, Castellón, E-12080, Spain
SOURCE: Anales de Química International Edition (1997), 93(4), 260-266
CODEN: AQIEFZ
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 79868-78-3DB, polymer-supported
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of polystyrene resins contg. chiral groups derived from amino acids)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

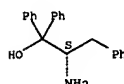
Absolute stereochemistry. Rotation (-).



AB Copper complexes of chiral pyridine bis(diphenyloxazoline)-type ligands have been studied as catalysts for the enantioselective allylic oxidn. of olefins. Using 2.5-5 mol % of these chiral catalysts and tert-Bu perbenzoate as oxidant, optically active allylic benzoates were obtained in up to 86% ee. A variety of copper salts was studied under different conditions and in different solvents. Acetone was found to be a superior solvent for the reaction. Use of phenylhydrazine in conjunction with the chiral copper complex played a crucial role in increasing the rate of the reaction. Use of 4 .ANG. mol. sieves increased the optical yield of product in almost every case.

ACCESSION NUMBER: 1998:253169 CAPLUS
DOCUMENT NUMBER: 128:230047
TITLE: Asymmetric Kharasch reaction: catalytic enantioselective allylic oxidation of olefins using chiral pyridine bis(diphenyloxazoline)-copper complexes and tert-butyl perbenzoate
AUTHOR(S): Sekar, Govindasamy; DattaGupta, Arpita; Singh, Vinod K.
CORPORATE SOURCE: Department of Chemistry, Indian Institute of Technology, Kanpur, 208016, India
SOURCE: Journal of Organic Chemistry (1998), 63(9), 2961-2967
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:230047
IT 79868-78-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective oxidn. of olefins to allylic benzoates with catalytic copper (I) bis(diphenyloxazoline) complexes and tert-Bu perbenzoate)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



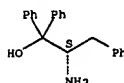
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

AB Title compds. I (R1, R2 = lower alkyl, aryl, aralkyl) are prepd. (2S)-2-amino-1,1-dibutyl-3-phenyl-1-propanol was treated with CS2 in the presence of KOH in EtOH/H2O under reflux for 7.5 h to give 394 (4S)-I (R1 = CH2Ph, R2 = Bu), which was used in anal. of flurbiprofen optical isomers.

ACCESSION NUMBER: 1997:442669 CAPLUS
DOCUMENT NUMBER: 127:50634
TITLE: Preparation of optically active 1,3-oxazolidine-2-thiones for optical purity determination
INVENTOR(S): Isobe, Toshio; Fukuda, Keiko; Takashi, Miho
PATENT ASSIGNEE(S): Shiratori Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JXOXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

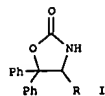
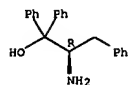
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09124621	A2	19970513	JP 1995-284824	19951101
PRIORITY APPLN. INFO.:			JP 1995-284824	19951101
OTHER SOURCE(S): MARPAT 127:50634				
IT 79868-78-3 86906-05-0				
RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. of optically active oxazolidinethiones for optical purity detn. of carboxylic acids)				
RN 79868-78-3 CAPLUS				
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)				

Absolute stereochemistry. Rotation (-).



RN 86906-05-0 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

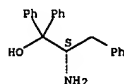


AB Title compds. I (R = alkyl, aryl, aralkyl), which are useful in selective prepn. of optically active compds. and are reusable, are prepd. (2S)-2-amino-1,1-diphenyl-1-propanol was treated with Et3N and N,N'-succinimidyl carbonate to give 87% (S)-I (R = Me).

ACCESSION NUMBER: 1997:435317 CAPLUS
DOCUMENT NUMBER: 127:50635
TITLE: Preparation of optically active 5,5-diphenyl-2-oxazolidinones as asymmetric agents
INVENTOR(S): Isobe, Toshio; Fukuda, Keiko
PATENT ASSIGNEE(S): Shiretori Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKOXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09143173	A2	19970603	JP 1995-301528	19951120
PRIORITY APPLN. INFO.:			JP 1995-301528	19951120
OTHER SOURCE(S): CASREACT 127:50635; MARPAT 127:50635				
IT 79868-78-3 86906-05-0				
RL: RCT (Reactant); RACT (Reactant or reagent)				
(prepn. of reusable optically active 5,5-diphenyl-2-oxazolidinones for asym. synthesis)				
RN 79868-78-3 CAPLUS				
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)				
(CA INDEX NAME)				

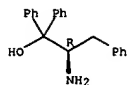
Absolute stereochemistry. Rotation (-).



RN 86906-05-0 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.R)- (9CI)

(CA INDEX NAME)

Absolute stereochemistry.



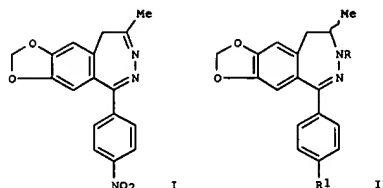
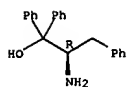
AB A process for prepg. optically active alcs. R1R2C*H2OH (I; R1, R2 = (un)substituted alkyl or aryl, or R1 and R2 cooperate to form a ring or heterocycle) are prepd. by reacting prochiral ketones with boron-contg. compds. such as borane compds. which are obtained from optically active .beta.-aminoalcs. and boron hydrides, optically active oxazaborolidines, and metal borohydrides in the presence of acids is claimed. A process for prepg. optically active amines R1R2C*HNH2 by reacting oxime derivs. with boron compds. is also claimed. These process increases optical purity effectively even in an industrial scale while using less amt. of boron compds. Thus, acetophenone was reduced by a mixt. of NaBH4 and (1S,2R)-(+)-norephedrine in the presence of H2SO4 to give 10.4% (R)-isomer

and 89.6% (S)-isomer of I (R1 = Ph, R2 = Me).

ACCESSION NUMBER: 1996:721585 CAPLUS
DOCUMENT NUMBER: 126:7684
TITLE: Processes for preparing optically active alcohols and optically active amines by selective asymmetric reduction of prochiral ketones and oximes
INVENTOR(S): Yoneyoshi, Yukio; Konya, Naoto; Suzukamo, Gohfu; Kamitani, Masafumi; Miyawaki, Takashi
PATENT ASSIGNEE(S): Sumitomo Chemical Company, Limited, Japan
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 736509	A2	19961009	EP 1996-105569	19960409
EP 736509	A3	19970319		
EP 736509	B1	20011114		
R: BE, CH, DE, FR, GB, IT, LI, NL				
JP 08333286	A2	19961217	JP 1996-69823	19960326
JP 08333309	A2	19961217	JP 1996-69824	19960326
JP 08337556	A2	19961224	JP 1996-69821	19960326
JP 09067284	A2	19970311	JP 1996-69822	19960326
US 5801280	A	19980901	US 1996-628154	19960405
US 6025531	A	20000215	US 1998-89349	19980603
PRIORITY APPLN. INFO.:			JP 1995-82913	A 19950407
			JP 1995-82920	A 19950407
			JP 1995-82958	A 19950407
			JP 1995-88450	A 19950413
			JP 1995-156071	A 19950622
			US 1996-628154	A3 19960405
OTHER SOURCE(S): CASREACT 126:7684; MARPAT 126:7684				
IT 86906-05-0, (R)-2-Amino-1,1,3-triphenyl-1-propanol				
RL: RCT (Reactant); RACT (Reactant or reagent)				
(processes for prepg. optically active alcs. and optically active amines by selective asym. redn. of prochiral ketones and oximes)				
RN 86906-05-0 CAPLUS				
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.R)- (9CI)				
(CA INDEX NAME)				

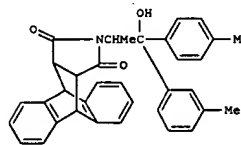
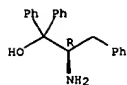
Absolute stereochemistry.



AB A highly specific enantioselective redn., elaborated for the redn. of the 3,4-carbon-nitrogen double bond of I, made possible the synthesis of the enantiomers of the potent noncompetitive AMPA/kainate antagonists II (R = Ac, CONHMe; R1 = NH2). E.g., a reducing complex prep. from (S)-(-)-2-amino-4-methyl-1,1-diphenyl-1-pentanol and BH3.THF was used to reduce I to give 68% (-)-II (R = H, R1 = NO2). NMR Investigations of the reducing complex show that there is no formation of an 1,3,2-oxazaborolidine ring as may have been presumed on the basis of literature data.

ACCESSION NUMBER: 1995:628706 CAPLUS
DOCUMENT NUMBER: 123:285961
TITLE: Asymmetric reduction of a carbon-nitrogen double bond:
enantioselective synthesis of 4,5-dihydro-3H-2,3-benzodiazepines
AUTHOR(S): Ling, Istvan; Podanyi, Benjamin; Hamori, Tamas; Solyom, Sandor
CORPORATE SOURCE: Inst. Drug Res. Lab., Budapest, H-1325, Hung.
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1995), (11), 1423-7
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:285961
IT 86906-05-0
RL: NUU (Other use, unclassified); USES (Uses)
(enantioselective synthesis of dihydrobenzodiazepines by asym. redn. of a carbon-nitrogen double bond)
RN 86906-05-0 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha., .alpha.-diphenyl-, (.beta.R)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

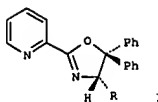
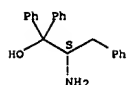


AB Cryst. host compds. consisting of a roof-shaped dicarboximide framework and pendant diarylethanol analogous subunits were synthesized and shown to form inclusion complexes with small org. mols. such as alcs., amines, ketones or polar and apolar org. solvents. Clathrate efficiency and selectivity depend on the particular host structure. The crystal and mol.

structures of a free host compd. (2S-I) and of inclusion compds. with 3-methylcyclohexanone, 3-methylcyclopentanone, 2-methylcyclohexanone, butyronitrile, propan-1-ol, and (-)-fenchone were detd. by x-ray diffraction anal. In all the structures, the hydroxyl group is involved in intramol. hydrogen bonds and the host and guest mols. are held by lattice forces only. The channels and cavities left in the host matrix are large enough to allow disorder or high thermal displacement parameters

of the guest mols. The local packing coeffs. for all guests are 0.cntdot.42 on av.
ACCESSION NUMBER: 1995:504923 CAPLUS
DOCUMENT NUMBER: 123:227567
TITLE: Dicarboximide-based clathrate design. Host synthesis, inclusion formation and X-ray crystal structures of a free host and of inclusion compounds with 2- and 3-methylcyclohexanone, 3-methylcyclopentanone, butyronitrile, propan-1-ol and (-)-fenchone guests
AUTHOR(S): Weber, Edwin; Reutel, Christiane; Foces-Foces, Concepcion; Llanas-Seiz, Antonio L.
CORPORATE SOURCE: Inst. Organische Chemie, Technischen Univ. Bergakademie Freiberg, Freiberg/Sachs, D-09596, Germany
SOURCE: Journal of Physical Organic Chemistry (1995), 8(3), 159-70
CODEN: JPOCEE; ISSN: 0894-3230
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 79868-78-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of dicarboximide-based host mols. and their clathrates)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha., .alpha.-diphenyl-, (.beta.S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

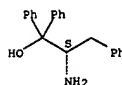


AB The 5,5-diphenyl-2-(2-pyridinyl)oxazolines [I; R=Me, PhCH₂, Me₂CH, Me₂CHCH₂, (S)-CHMeEt] give ee values 9.6-34.2% higher than their unsubstituted counterparts in the Rh-catalyzed enantioselective hydrosilylation of acetophenone with diphenylsilane.

ACCESSION NUMBER: 1995:504063 CAPLUS
DOCUMENT NUMBER: 123:111616
TITLE: Enantioselective catalysis. 94. The "diphenyl effect" in the enantioselective hydrosilylation of acetophenone with diphenylsilane using Rh/5,5-diphenyl-2-(2-pyridinyl)oxazoline catalysts

AUTHOR(S): Burmner, Henri; Henrichs, Christopher
CORPORATE SOURCE: Institut fuer Anorganische Chemie, Universitaet Regensburg, Regensburg, D-93040, Germany
SOURCE: Tetrahedron: Asymmetry (1995), 6(3), 653-6
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:111616
IT 79868-78-3
RL: RCT (Reactant); RACT (Reactant or reagent) (enantioselective hydrosilylation of acetophenone with diphenylsilane using Rh/5,5-diphenyl-2-(2-pyridinyl)oxazoline catalysts)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

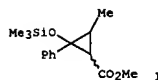
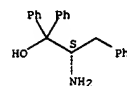
Absolute stereochemistry. Rotation (-).



L4 ANSWER 27 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
AB Nine new optically active N,N-dialkyl-.beta.-amino alcs. synthesized from natural amino acids reacted with borane in THF to give chiral oxazaborolidines. The borane modified by chiral oxazaborolidines enantioselectively reduced aliph. and arom. ketones to yield sec-alcs. with 100% yield and medium to high optical yields. Some influences of steric effect, reaction temp. and solvent effects were discussed.

ACCESSION NUMBER: 1995:436355 CAPLUS
DOCUMENT NUMBER: 123:285402
TITLE: Asymmetric reduction of Ketones using optically active
active
N,N-dialkyl-.beta.-amino alcohol-borane complexes
AUTHOR(S): Zhao, Jun; Zhou, Wang-Yue; Yang, Shi-Yan; Jin Dao-Sen
CORPORATE SOURCE: Dep. Chem. Eng., Zhejiang Univ. Technology, Hangzhou, 310014, Peop. Rep. China
SOURCE: Youji Huaxue (1995), 15(1), 39-46
CODEN: YCHMDX; ISSN: 0253-2786
PUBLISHER: Kexue
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
IT 79868-78-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (asym. redn. of ketones using optically active N,N-dialkyl-.beta.-amino alc.-borane complexes)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

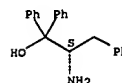


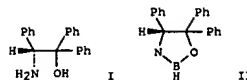
AB The cyclopropanation of silyl enol ether Me₃SiOC(Ph):CHMe 1a with Me diazoacetate (2a) and diazo esters in the presence of optically active copper silylimine complexes was systematically studied. Up to 88% enantiomeric excess in products 3 were obtained by employing the appropriate reaction conditions and the optimal catalyst ligands. Thus, for the first time respectable optical yields were achieved in asym. cyclopropanations of silyl enol ethers with easily available copper-Schiff base catalysts. The ring opening of the sepd. diastereomers of 3a (shown as I) employing Bu₄NF provided Me .gamma.-oxo-carboxylate PhCOCHMeCH₂CO₂Me 6a in good optical purity. This demonstrates that this process occurs without racemization and also that 3a is formed with the same abs. configuration at C-1.

ACCESSION NUMBER: 1994:298674 CAPLUS
DOCUMENT NUMBER: 120:298674
TITLE: Synthesis of optically active siloxycyclopropanes by asymmetric catalysis. I. Influence of the catalyst on the cyclopropanation of (Z)-1-phenyl-1-(trimethylsiloxy)prop-1-ene

AUTHOR(S): Dumast, Franziska; Reissig, Hans Ulrich
CORPORATE SOURCE: Inst. Org. Chem., Tech. Hochsch. Darmstadt, Darmstadt, D-64287, Germany
SOURCE: Chemische Berichte (1993), 126(11), 2449-56
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 120:298674
IT 79868-78-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and reaction of, with salicylaldehyde deriv.)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

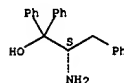




AB Enantiocontrolled redn. of prochiral ketones, e.g., acetophenone, with borane in the presence of homochiral amino alcs., e.g., I, forming a oxazaborolidine intermediate, e.g., II, as the enantioselective catalysts afforded the chiral corresponding secondary alcs. in moderate to high (55 to 88%) optical yields.

ACCESSION NUMBER: 1994:106465 CAPLUS
DOCUMENT NUMBER: 120:106465
TITLE: Enantioselective catalytic borane reductions of achiral ketones: synthesis and application of new rigid catalysts prepared from (R)-phenylglycine and (S)-phenylalanine
AUTHOR(S): Dauelsberg, C.; Martens, J.
CORPORATE SOURCE: Fachbereich Chem., Univ. Oldenburg, Oldenburg, 2900, Germany
SOURCE: Synthetic Communications (1993), 23(15), 2091-9
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:106465
IT 79868-78-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with borane, oxazaborolidine from as enantioselective redn. catalyst for ketones)
RN 79868-78-3 CAPLUS
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



=> fil reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	237.44	385.80
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
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 DICTIONARY FILE UPDATES: 4 NOV 2003 HIGHEST RN 612801-40-8

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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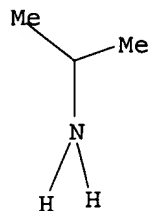
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
 PROPERTIES for more information. See STNote 27, Searching Properties
 in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>
 Uploading 09857465.str

L5 STRUCTURE UPLOADED

=> d query
 L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15
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 SAMPLE SCREEN SEARCH COMPLETED - 141655 TO ITERATE

0.7% PROCESSED	1000 ITERATIONS	9 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)		
SEARCH TIME: 00.00.01		

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 23356

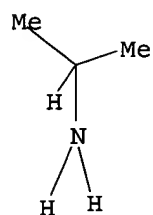
L6 9 SEA SSS SAM L5

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L7 STRUCTURE UPLOADED

=> d query

L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 17
SAMPLE SEARCH INITIATED 16:51:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 141655 TO ITERATE

0.7% PROCESSED 1000 ITERATIONS 1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 2119

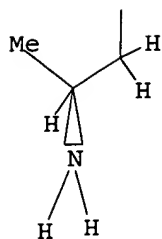
L8 1 SEA SSS SAM L7

=>
Uploading 09857465.str

L9 STRUCTURE UPLOADED

=> d query

L9 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 19

SAMPLE SEARCH INITIATED 16:52:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 98610 TO ITERATE

1.0% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 0

L10 0 SEA SSS SAM L9

=> s 19 full

FULL SEARCH INITIATED 16:53:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 20.3% PROCESSED 400000 ITERATIONS 91 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.11

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 384

L11 91 SEA SSS FUL L9

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	150.95	536.75
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-32.55

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FILE COVERS 1907 - 5 Nov 2003 VOL 139 ISS 19
FILE LAST UPDATED: 4 Nov 2003 (20031104/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l11
L12

45 L11

=> d l12 30-45 abs ibib hitstr

L12 ANSWER 30 OF 45 CAPLUS COPYRIGHT 2003 ACS ON STN
AB Zwitterionic dipeptides have recently been shown to exist in water mainly
as nine conformational forms with specific combinations of backbone

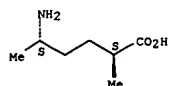
.psi., .omega. and .vphi. torsions, which allows conformer-specific mol.
recognition of peptide ligands by proteins. Here, the authors show that
pairs of virtual backbone torsions can also define these nine
conformational forms, and that comparing these virtual torsions in
dipeptides with those of backbone-modified pseudopeptides offers an
improved procedure for evaluating peptidomimetics for therapeutic
applications.

ACCESSION NUMBER: 2002:325926 CAPLUS
DOCUMENT NUMBER: 137:93990
TITLE: Presence of distinct virtual backbone torsion angles
in dipeptide conformers
AUTHOR(S): Gupta, S.; Grail, B. M.; Payne, J. W.
CORPORATE SOURCE: School of Biological Sciences, University of Wales
Bangor, Bangor, LL57 2UW, UK
SOURCE: Protein and Peptide Letters (2002), 9(2), 133-138
CODEN: PPELEN; ISSN: 0929-8665
PUBLISHER: Bentham Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

IT 425644-63-9
RL: PRP (Properties)
(mol. modeling of the backbone torsion angles in alanyl
pseudodipeptide
conformers)

RN 425644-63-9 CAPLUS
CN Hexanoic acid, 5-amino-2-methyl-, (2S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



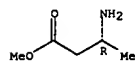
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR
THIS
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

L12 ANSWER 31 OF 45 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)
EP 1326838 A1 20030716 EP 2001-979459 20011004
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
PRIORITY APPLN. INFO.: US 2000-238316P P 20001005
GB 2001-8903 A 20010410
WO 2001-US31087 W 20011004

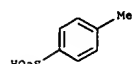
IT 409081-18-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant: prepn. of cryst. forms of factor Xa inhibitor Me
(2R,3R)-2-[3-(amidinobenzyl)-3-[(4-(1-oxido-4-
pyridinyl)benzoyl]amino]butanoate)
RN 409081-18-1 CAPLUS
CN Butanoic acid, 3-amino-, methyl ester, (3R)-, 4-methylbenzenesulfonate
(9CI) (CA INDEX NAME)

CM 1
CRN 103189-63-5
CMF C5 H11 N O2

Absolute stereochemistry.

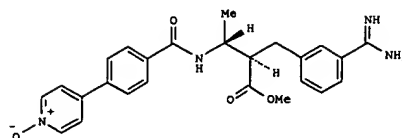


CM 2
CRN 104-15-4
CMF C7 H9 O3 S



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
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L12 ANSWER 31 OF 45 CAPLUS COPYRIGHT 2003 ACS ON STN
GI



AB I hydrochloride, 2-butanol hemisolvate was prepd. in cryst. form.
(R)-3-aminobutanoic acid Me ester p-toluenesulfonate was alkylated with
3-cyanobenzyl bromide (THF, LHMDS, -20.degree.C) and the product
condensed
with the corresponding biaryl carboxylic acid (DMF, TBTU, NMM) and the
resulting pyridine oxidized (CH2Cl2/H2O, MPPF) and then hydrolyzed (MeOH,
HCl, NH3, -5.degree.C) to give amidine I as the hydrochloride salt (with
NH4Cl as a solid byproduct). I.bul.HCl was dissolved in 2-butanol at
70.degree.C and the NH4Cl removed by filtration. The resulting filtrate
was seeded and cooled to afford a ppt. which was filtered at
-15.degree.C,
rinsed with 2-butanol and dried at 45-50.degree.C. The resulting
I.bul.HCl, 2-butanol hemisolvate (II) was characterized by 1H/13C-NMR,
DSC, elemental anal., MS and by X-ray powder diffraction. II is a factor
Xa inhibitor useful for the treatment of acute myocardial infarction,
unstable angina, thromboembolism, etc.

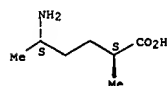
ACCESSION NUMBER: 2002:275967 CAPLUS
DOCUMENT NUMBER: 136:294740
TITLE: Preparation of crystalline forms of factor Xa
inhibitor methyl
(2R,3R)-2-[3-(amidinobenzyl)-3-[(4-(1-
oxido-4-pyridinyl)benzoyl]amino]butanoate
INVENTOR(S): Woodward, Rick G.; Teager, David S.
PATENT ASSIGNEE(S): Aventis Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXKD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002028936	A1	20020411	WO 2001-US31087	20011004
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RW:	GH, GM, KE, LS, MW, ML, SD, SL, SE, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2002011425	A5	20020415	AU 2002-11425	20011004

L12 ANSWER 32 OF 45 CAPLUS COPYRIGHT 2003 ACS ON STN
AB Our aim was to compare the repertoires of conformers formed by the model
zwitterionic peptides AA and AAA in aq. soln. with the conformational
profiles of a range of their peptide isosteres, so as to facilitate
selection of isosteres for synthesis and testing as biol. stable
surrogates of bioactive di- and tripeptides. Comparison: were based upon
the results of conformational anal. using a random search approach
implemented within the SYBYL mol. modelling package, using zwitterionic
mols., simulated aq. solvation using a dielec. const. of 80 and allowing
all torsions to vary. For each compd., individual conformers were
grouped
on the basis of specific combinations of psi, phi and omega torsions and,
using their energies, the aggregated percentage for each group was calcd.
using a Boltzmann distribution and displayed using a 3D pseudo
Ramachandran plot relating percentage conformer to psi and phi torsions.
Retroamide, N-methylamide and thioamide isosteres showed the best match
to
natural peptides and to the mol. recognition parameters defined for
substrates of peptide transporters. The results should aid rational
design of therapeutic agents in various areas, e.g. oral delivery of
drugs
by peptide transporters and of peptidase inhibitors. This approach may
usefully be applied to various biochem. and pharmaceutical topics.

ACCESSION NUMBER: 2002:203449 CAPLUS
DOCUMENT NUMBER: 136:386389
TITLE: Evaluation of the conformational propensities of
peptide isosteres as a basis for selecting bioactive
pseudopeptides
AUTHOR(S): Gupta, S.; Payne, J. W.
CORPORATE SOURCE: School of Biological Sciences, University of Wales
Bangor, Bangor, LL57 2UW, UK
SOURCE: Journal of Peptide Research (2001), 58(6), 546-561
CODEN: JPERFA; ISSN: 1397-002X
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 425644-63-9
RL: PRP (Properties)
(evaluation of the conformational propensities of peptide isosteres as
a basis for selecting bioactive pseudopeptides)
RN 425644-63-9 CAPLUS
CN Hexanoic acid, 5-amino-2-methyl-, (2S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR
THIS
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A series of eleven .alpha.-aminoacyl stabilized phosphorus ylides, e.g., I, have been prep'd. by condensation of N-alkoxycarbonyl protected amino acids with Ph3P:CHCO2Et using a carbodiimide peptide coupling reagent. Upon flash vacuum pyrolysis at 600 .degree.C, these undergo extrusion of Ph3PO to give the corresponding .alpha.,.beta.-acetylenic .gamma.-amino esters II [R1= Bn, R2 = Me, 1-Pr, 1-Bu; R1 = Et, R2 = H, Me, 1-Pr, 1-Bu, sec-Bu; R1 = 1-Bu, R2 = Me] and III [R1 = Bn, Et] in moderate yield. In two cases terminal alkynes were also formed. The .beta.-aminoacyl ylide IV from .beta.-alanine similarly gives the .alpha.,.beta.-acetylenic .delta.-amino ester V upon pyrolysis. Regioselective addn. of HBr to the triple bond of one acetylenic ester II [R1 = Et, R2 = Me] was obsd.

giving a mixt. of E and Z .alpha.-bromoacrylates. Hydrogenation of the N-Cbz acetylenic esters II [R1 = Bn; R2 = Me, 1-Pr, 1-Bu] and III [R1 = Bn] results in N-deprotection and hydrogenation of the triple bond to afford the chiral GABA analogs VI [R2 = Me, 1-Pr, 1-Bu] and VII in 70 ->95% ee

as detd. by 19F NMR of their Mosher amides. Fully assigned 13C NMR spectra of all the ylides and acetylenic ester deriva. are presented.

ACCESSION NUMBER: 2002:133700 CAPLUS

DOCUMENT NUMBER: 137:79192

TITLE: Flash vacuum pyrolysis of stabilized phosphorus ylides. Part 17.1 Preparation of aliphatic amino acid derived .gamma.-alkoxycarbonylamino-.beta.-oxo ylides and pyrolysis to give .alpha.,.beta.-acetylenic .gamma.-amino acid and GABA analogues

AUTHOR(S): Aitken, R. Alan; Karodia, Nazira; Massil, Tracy; Young, Robert J.

CORPORATE SOURCE: School of Chemistry, University of St. Andrews, North Haugh, Fife, St. Andrews, KY16 9ST, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1

(2002), (4), 533-541

CODEN: JCSPCE; ISSN: 1472-7781

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:79192

IT 441012-57-3P

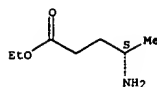
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(stereoselective prepn. of aliph. amino acid derived .gamma.-alkoxycarbonylamino-.beta.-oxo ylides and pyrolysis to give .alpha.,.beta.-acetylenic .gamma.-amino acid and GABA analogs)

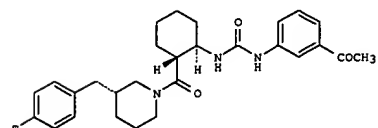
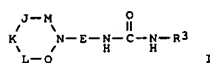
RN 441012-57-3 CAPLUS

CN Pentanoic acid, 4-amino-, ethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



AB Title compds. I [M = absent CH2, CHR5, CHR13, CR13R13, and CR5R13; Q = CH2, CHR5, CHR13, CR13R13, and CR5R13; K = CH2, CHR5 and CHR6; J, L = CH2, CHR5, CHR6, CR6R6 and CR5R6; with the provisions that at least one of M, J, K, L, or Q contains an R5; and when M absent, J = CH2, CHR5, CHR13 and CR5R13; Z = O, S, NR1a, C(CN)2, CH(NO)2, CHCN; R1a = H, (cyclo)alkyl, amido, alkoxy, CN, NO2, etc.; E = C=O-alkyl, sulfonyl-alkyl, C=O-cycloalkyl, etc.; R3 = alkylamino, alkyl-carbocyclic, etc.; R5 = alkyl-carbocyclic; R6 = alk(en/yn)yl, alkyl-cycloalkyl, CN, alkylamino, alkyl-hydroxy, etc.; R13 = alk(en/yn)yl, cycloalkyl, alkyl-CF3, alkylamino, alkyl-alkoxy, etc.] were prep'd. Over 80 synthetic examples were disclosed. For instance,

(1R,2R)-2-(benzyloxycarbonylamino)cyclohexanecarboxaldehyde (prepn. given) was oxidized to the corresponding carboxylic acid (NaOAc/HOAc, pH 3.5, CH3CN, resorcinol, NaClO2, 0.degree.C, 16 h) and condensed with (S)-3-(4-fluorobenzyl)piperidine (prepn. given: CH2Cl2, BOP, Et3N, 0.degree.C, 16 h) to give the amide. The intermediate Cbz group was removed (MeOH, 10% Pd/C, 50 psi H2, overnight) and the amine acylated with 3-acetylphenylisocyanate (THF, 25.degree.C) to give example compd. II. I are modulators of chemokine receptor activity and are useful in the prevention of asthma and other allergic diseases.

ACCESSION NUMBER: 2001:935573 CAPLUS

DOCUMENT NUMBER: 136:53686

TITLE: Synthesis of piperidine-amido-ureas as modulators of chemokine receptor activity

INVENTOR(S): Duncia, John V.; Santella, Joseph B.; Wacker, Dean A.;

Yao, Wenqing; Zheng, Changsheng

PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA

SOURCE: PCT Int. Appl., 326 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001098268	A2	20011227	WO 2001-US19705	20010620
WO 2001098268	A3	20020808		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TH, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 2002156102	A1	20021024	US 2001-885550	20010620
US 6638950	B2	20031028		
EP 1296949	A2	20030402	EP 2001-946580	20010620
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
PRIORITY APPLN. INFO.:			US 2000-213066P	P 20000621
			WO 2001-US19705	W 20010620

OTHER SOURCE(S): MARPAT 136:53686

IT 382638-02-0P

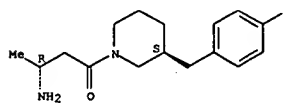
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; synthesis of piperidine amides as modulators of chemokine receptor activity)

RN 382638-02-0 CAPLUS

CN Piperidine, 1-[(3R)-3-amino-1-oxobutyl]-3-[(4-fluorophenyl)methyl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 35 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN
 AB Intense efforts of research are made for developing antitumor vaccines that stimulate T cell-mediated immunity. Tumor cells specifically express at their surfaces antigenic peptides presented by MHC class I and recognized by CTL. Tumor antigenic peptides hold promise for the development of novel cancer immunotherapies. However, peptide-based vaccines face two major limitations: the weak immunogenicity of tumor Ags and their low metabolic stability in biol. fluids. These two hurdles, for which sep. solns. exist, must, however, be solved simultaneously for developing improved vaccines. Unfortunately, attempts made to combine increased immunogenicity and stability of tumor Ags have failed until now.

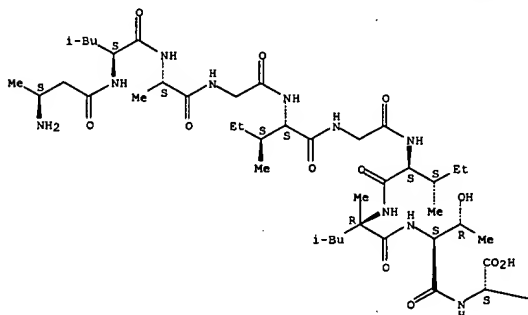
Here the authors report the successful design of synthetic derivs. of the human tumor Ag Melan-A/MART-1 that combine for the first time both higher immunogenicity and high peptidase resistance. A series of 36 nonnatural peptide derivs. was rationally designed on the basis of knowledge of the mechanism of degradn. of Melan-A peptides in human serum and synthesized. Eight of them were efficiently protected against proteolysis and retained the antigenic properties of the parental peptide. Three of the eight analogs were twice as potent as the parental peptide in stimulating in vitro Melan-specific CTL responses in PBMC from normal donors. The authors isolated these CTL by tetramer-guided cell sorting and expanded them in vitro. The resulting CTL efficiently lysed tumor cells expressing Melan-A Ag. These Melan-A/MART-1 Ag derivs. should be considered as a new generation of potential immunogens in the development of mol. anti-melanoma vaccines.

ACCESSION NUMBER: 2001:832584 CAPLUS
 DOCUMENT NUMBER: 136:117005
 TITLE: A new generation of Melan-A/MART-1 peptides that fulfill both increased immunogenicity and high resistance to biodegradation: implication for molecular anti-melanoma immunotherapy
 AUTHOR(S): Blanchet, Jean-Sebastien; Valmori, Danila; Dufau, Isabelle; Ayyoub, Maha; Nguyen, Christophe; Guillaume, Philippe; Monsarrat, Bernard; Cerottini, Jean-Charles; Romero, Pedro; Gairin, Jean Edouard
 CORPORATE SOURCE: Laboratoire d'Immunopharmacologie Structurale, Institut de Pharmacologie et Biologie Structurale, Centre National de la Recherche Scientifique, Toulouse, 31400, Fr.
 SOURCE: Journal of Immunology (2001), 167(10), 5852-5861
 PUBLISHER: American Association of Immunologists
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 IT 390817-89-7P 390817-90-0P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (new generation of Melan-A/MART-1 peptides that fulfill both increased immunogenicity and high resistance to biodegradn.)
 RN 390817-89-7 CAPLUS
 CN L-Valine, N-[(1S)-3-amino-1-oxobutyl]-L-leucyl-L-alanylglycyl-L-isoleucylglycyl-L-isoleucyl-2-methyl-L-leucyl-L-threonyl- (9CI) (CA
 INDEX

L12 ANSWER 35 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 INDEX isoleucylglycyl-L-isoleucyl-2-methyl-D-leucyl-L-threonyl- (9CI) (CA
 NAME)

Absolute stereochemistry.

PAGE 1-A

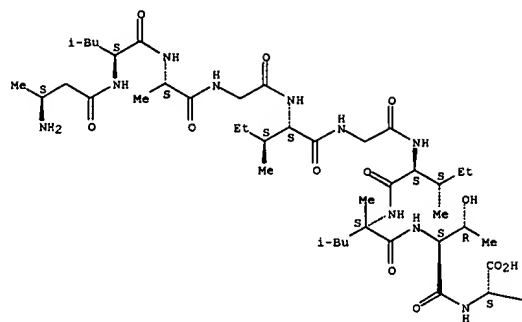


PAGE 1-B

L12 ANSWER 35 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

Pr-i

RN 390817-90-0 CAPLUS
 CN L-Valine, N-[(1S)-3-amino-1-oxobutyl]-L-leucyl-L-alanylglycyl-L-

L12 ANSWER 35 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

Pr-i

L12 ANSWER 36 OF 45 CAPLUS COPYRIGHT 2003 ACS ON STN

AB One- and two-color, mass selected R2PI spectra of the S1.rar.S0 transitions in the bare (+)-(R)-1-phenyl-1-ethanol (ER) and its complexes with different solvent mol. (solv) (-)-(R)-2-butanol (BR) or (+)-(S)-2-butanol (BS) and (-)-(R)-2-butylamine (AR) or (+)-(S)-2-butylamine (AS), have been recorded after a supersonic mol.

beam expansion. The one-color R2PI excitation spectra of the diastereomeric complexes are characterized by significant shifts of their band origin relative to that of bare ER. The extent and the direction of these spectral shifts are found to depend on the structure and the configuration of solv and are attributed to different short-range interactions in the ground and excited states of the complexes. In analogy with other diastereomeric complexes, the phenomenon. binding energy of the

homochiral cluster is found to be greater than that of the heterochiral one.

ACCESSION NUMBER: 2001:832185 CAPLUS
DOCUMENT NUMBER: 136:150869
TITLE: R2PI study of intermolecular hydrogen bond in solvent-free chiral complexes
AUTHOR(S): Guidoni, A. Giardini, Piccirillo, S.; Scuderi, D.; Satta, M.; Di Palma, T. M.; Speranza, M.; Filippi, A.;

A.: Paladini, A.
CORPORATE SOURCE: Dipartimento di Chimica, Universita' di Roma "La Sapienza", Rome, I-00185, Italy
SOURCE: Chirality (2001), 13(10), 727-730
CODEN: CHRLEP; ISSN: 0899-0042
PUBLISHER: Wiley-Liss, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

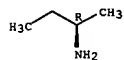
IT 389140-16-3 389140-17-4
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (R2PI study of intermol. hydrogen bond in solvent-free chiral complexes)

RN 389140-16-3 CAPLUS
CN Benzenemethanol, .alpha.-methyl-, (.alpha.R)-, compd. with (2R)-2-butylamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 13250-12-9
CMF C4 H11 N

Absolute stereochemistry. Rotation (-).



CM 2

CRN 1517-69-7
CMF C8 H10 O

L12 ANSWER 37 OF 45 CAPLUS COPYRIGHT 2003 ACS ON STN

AB Discrimination of chiral amines by dimethyldiketopyridino-18-crown-6 (1) is studied by free energy perturbation (FEP) and mol. dynamics (MD) methods. 1 Has two (S)-chiral centers and discriminates chiral amines through host-guest interactions. The optically active amines in this study are .alpha.-(1-naphthyl)ethylamine, methylbenzylamine, cyclohexylethylamine, and sec-butylamine. The trends in binding free energy differences obtained from FEP calcs. were in excellent agreement with exptl. results obtained in the gas phase. In order to explain the enantioselectivity of the host in terms of the host-guest interactions at the mol. level, we analyzed the structures generated by 10-ns MD simulations of host-guest complexes. The suggested chiral discrimination mechanism, the .pi.-.pi. interaction and the steric repulsion between the guest and the host, was verified by our MD simulation anal.

ACCESSION NUMBER: 2001:764099 CAPLUS
DOCUMENT NUMBER: 136:69482

TITLE: Free energy perturbation and molecular dynamics simulation studies on the enantiomeric discrimination of amines by dimethyldiketopyridino-18-crown-6
AUTHOR(S): Lee, One-Sun; Hwang, Sungu; Chung, Doo Soo
CORPORATE SOURCE: Department of Chemistry, Seoul National University, Seoul, 151-742, S. Korea
SOURCE: Supramolecular Chemistry (2000), 12(3), 255-272
CODEN: SCHEER; ISSN: 1061-0278
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

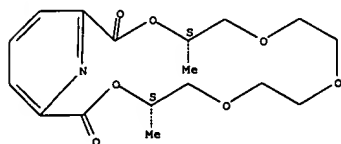
IT 384365-65-5 384365-67-7
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); FORM (Formation, nonpreparative); PROC (Process) (free energy perturbation and mol. dynamics simulation studies on the enantiomeric discrimination of amines by dimethyldiketopyridino-18-crown-6)

RN 384365-65-5 CAPLUS
CN 3,6,9,12,15-Pentaoxa-21-azabicyclo[15.3.1]heneicosa-1(21),17,19-triene-2,16-dione, 4,14-dimethyl-, (4S,14S)-, compd. with (2R)-2-butylamine (1:1), conjugate monoacid (9CI) (CA INDEX NAME)

CM 1

CRN 82468-65-3
CMF C17 H23 N O7

Absolute stereochemistry.



CM 2

L12 ANSWER 36 OF 45 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)
Absolute stereochemistry. Rotation (+).



RN 389140-17-4 CAPLUS
CN Benzenemethanol, .alpha.-methyl-, (.alpha.R)-, compd. with (2S)-2-butylamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 1517-69-7
CMF C8 H10 O

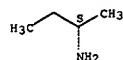
Absolute stereochemistry. Rotation (+).



CM 2

CRN 513-49-5
CMF C4 H11 N

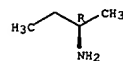
Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 37 OF 45 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)
CRN 13250-12-9
CMF C4 H11 N

Absolute stereochemistry. Rotation (-).

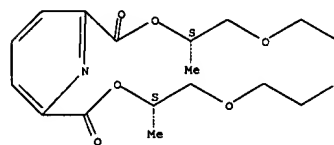


RN 384365-67-7 CAPLUS
CN 3,6,9,12,15-Pentaoxa-21-azabicyclo[15.3.1]heneicosa-1(21),17,19-triene-2,16-dione, 4,14-dimethyl-, (4S,14S)-, compd. with (2S)-2-butylamine (1:1), conjugate monoacid (9CI) (CA INDEX NAME)

CM 1

CRN 82468-65-3
CMF C17 H23 N O7

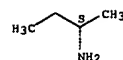
Absolute stereochemistry.



CM 2

CRN 513-49-5
CMF C4 H11 N

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 38 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN
 AS The study aims to det. whether .beta.-peptides in general and amphiphilic peptides in particular are antimicrobial and cytotoxic. Antimicrobial activity was examd. by incubating .beta.-peptides of various concns. (10, 20, 50 .mu.g) with 13 different eukaryotic and prokaryotic microorganisms.

All .beta.-peptides showed induction of arial mycelium formation and fructification of Cladosporium elatum and Penicillium claviformae, and most .beta.-peptides also stimulated growth of Aspergillus niger. The .beta.-peptides were also tested for hemolytic activity. In almost all cases, the activity was low (.ltoreq.5%), with the exception of dodecapeptide (15%). The results suggested that .beta.-peptides in general are not dangerous cytotoxic compds., and that activity and selectivity of amphiphilic peptides and their analogs are critically dependent on the side-chain compn. of the helix.

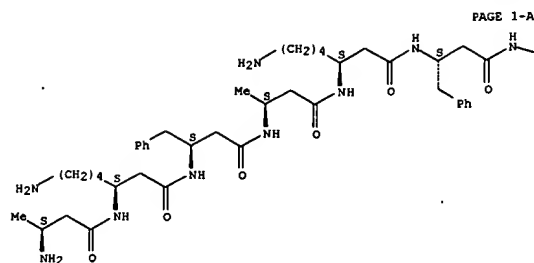
ACCESSION NUMBER: 2001:752804 CAPLUS
 DOCUMENT NUMBER: 136:02497
 TITLE: On the antimicrobial and hemolytic activities of amphiphilic .beta.-peptides
 AUTHOR(S): Arvidsson, Per I.; Frackepohl, Jens; Ryder, Neil S.; Liechty, Brigitta; Petersen, Frank; Zimmermann, Heidrun; Camenisch, Gian P.; Woessner, Ralph;

Seebach,
 CORPORATE SOURCE: Dieter
 Lab. Organische Chemie der Eidgenossischen Tech.
 Hochschule, ETH Zentrum Univ., Zurich, 8092, Switz.
 SOURCE: ChemBioChem (2001), 2(10), 771-773
 CODEN: CBCHFX; ISSN: 1439-4227

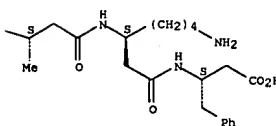
PUBLISHER: Wiley-VCH Verlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 IT 387339-12-0 387339-15-3 387339-17-5
 387339-18-6 387339-19-7 387339-20-0
 387339-21-1 387339-23-3
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
 BIOL (Biological study)
 (on antimicrobial and hemolytic activities of amphiphilic .beta.-peptides)
 RN 387339-12-0 CAPLUS
 CN 4, 8, 12, 16, 20, 24, 28, 32-Octaazahexatriacontanoic acid, 35-amino-7, 19, 31-tris(4-aminobutyl)-11, 23-dimethyl-5, 9, 13, 17, 21, 25, 29, 33-octaexo-3, 15, 27-tris(phenylmethyl)-, trihydrochloride,
 (3S, 7S, 11S, 15S, 19S, 23S, 27S, 31S, 35S)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 38 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



● 3 HCl



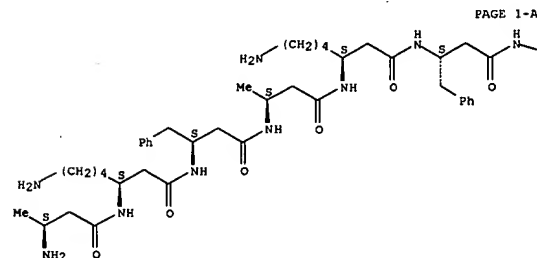
RN 387339-15-3 CAPLUS
 CN 4, 8, 12, 16, 20, 24, 28, 32-Octaazahexatriacontanoic acid, 35-amino-7, 19, 31-tris(4-aminobutyl)-11, 23-dimethyl-5, 9, 13, 17, 21, 25, 29, 33-octaexo-3, 15, 27-tris(phenylmethyl)-, (3S, 7S, 11S, 15S, 19S, 23S, 27S, 31S, 35S)-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

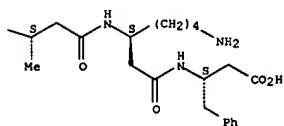
CRN 219967-57-4
 CMF C63 H98 N12 O10

Absolute stereochemistry.

L12 ANSWER 38 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



PAGE 1-B



CM 2

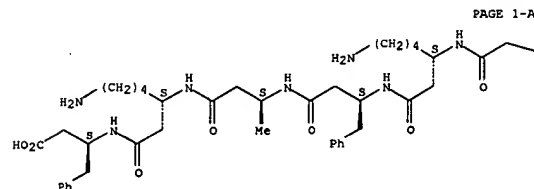
CRN 76-05-1
 CMF C2 H F3 O2



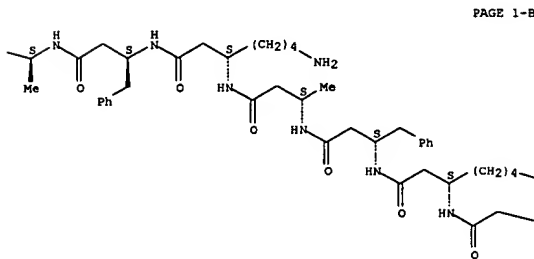
RN 387339-17-5 CAPLUS
 CN 4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 44-Undecaazaoctatetracontanoic acid, 47-amino-7, 19, 31, 43-tetrakis(4-aminobutyl)-4, 23, 35-trimethyl-5, 9, 13, 17, 21, 25, 29, 33, 37, 41, 45-undecaexo-3, 15, 27, 39-tetrakis(phenylmethyl)-, tetrahydrochloride, (3S, 7S, 11S, 15S, 19S, 23S, 27S, 31S, 35S, 39S, 43S, 47S)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 38 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)



● 4 HCl



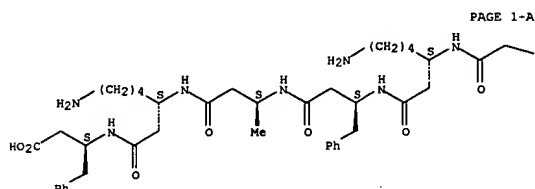


RN 387339-18-6 CAPLUS
 CN 4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 44-Undecaazaoctatetracontanoic acid,
 47-amino-7, 19, 31, 43-tetrakis(4-aminobutyl)-4, 23, 35-trimethyl-
 5, 9, 13, 17, 21, 25, 29, 33, 37, 41, 45-undecaoxo-3, 15, 27, 39-tetrakis(phenylmethyl)-
 , (3S, 7S, 11S, 15S, 19S, 23S, 27S, 31S, 35S, 39S, 43S, 47S)-,
 tetrakis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 336184-02-2
 CHF C84 H130 N16 O13

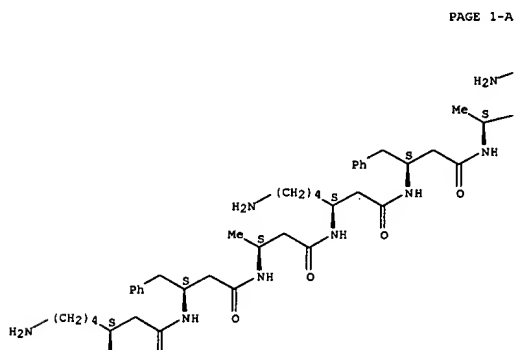
Absolute stereochemistry.



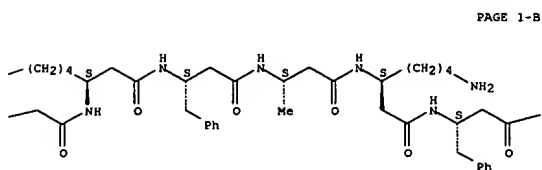
PAGE 1-A

L12 ANSWER 38 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 acid, 58-amino-6, 18, 30, 42, 54-pentakis(4-aminobutyl)-10, 22, 34, 46-
 tetramethyl-4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 44, 48, 52, 56-tetradeca-oxo-
 2, 14, 26, 38, 50-pentakis(phenylmethyl)-, pentahydrochloride,
 (2S, 6S, 10S, 14S, 18S, 22S, 26S, 30S, 34S, 38S, 42S, 46S, 50S, 54S, 58S)- (9CI) (CA
 INDEX NAME)

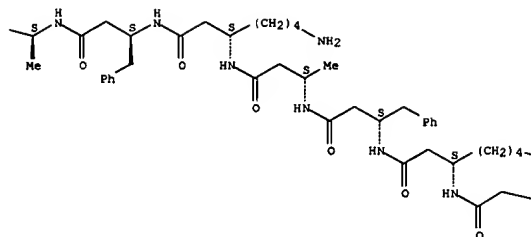
Absolute stereochemistry.



PAGE 1-A



PAGE 1-B



PAGE 1-C

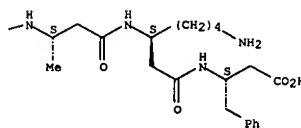


CM 2

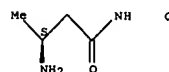
CRN 76-05-1
 CHF C2 H F3 O2



RN 387339-19-7 CAPLUS
 CN 3, 7, 11, 15, 19, 23, 27, 31, 35, 39, 43, 47, 51, 55-Tetradecaazanonapentacontanoic



PAGE 2-A



● 5 HCl

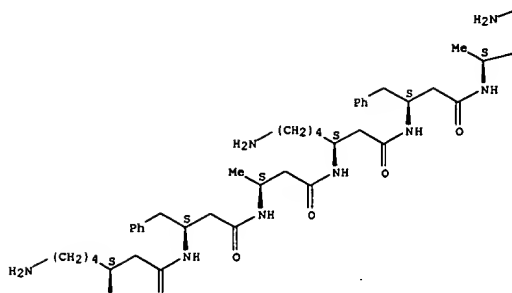
RN 387339-20-0 CAPLUS
 CN 3, 7, 11, 15, 19, 23, 27, 31, 35, 39, 43, 47, 51, 55-Tetradecaazanonapentacontanoic
 acid, 58-amino-6, 18, 30, 42, 54-pentakis(4-aminobutyl)-10, 22, 34, 46-
 tetramethyl-4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 44, 48, 52, 56-tetradeca-oxo-
 2, 14, 26, 38, 50-pentakis(phenylmethyl)-,
 (2S, 6S, 10S, 14S, 18S, 22S, 26S, 30S, 34S,
 38S, 42S, 46S, 50S, 54S, 58S)-, pentakis(trifluoroacetate) (9CI) (CA INDEX
 NAME)

CM 1

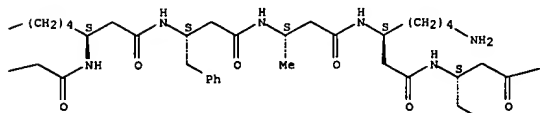
CRN 356783-64-7
 CHF C105 H162 N20 O16

Absolute stereochemistry.

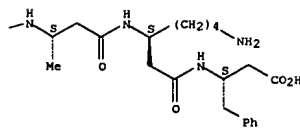
PAGE 1-A



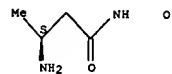
PAGE 1-B



PAGE 1-C



PAGE 2-A



CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 387339-21-1 CAPLUS

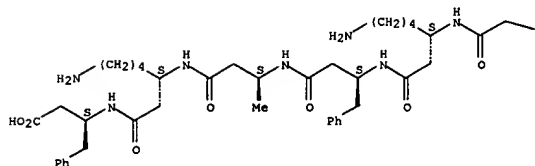
CN 4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 44, 48, 52, 56, 60, 64, 68-

Heptadecaazadoheptacontanoic acid, 71-amino-7, 19, 31, 43, 55, 67-hexakis(4-

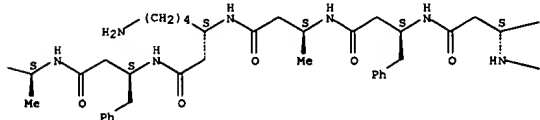
aminobutyl)-11, 23, 35, 47, 59-pentamethyl-5, 9, 13, 17, 21, 25, 29, 33, 37, 41, 45, 49, 53, 57, 61, 65, 69-heptadecaazo-3, 15, 27, 39, 51, 63-hexakis(phenylmethyl)-, hexahydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

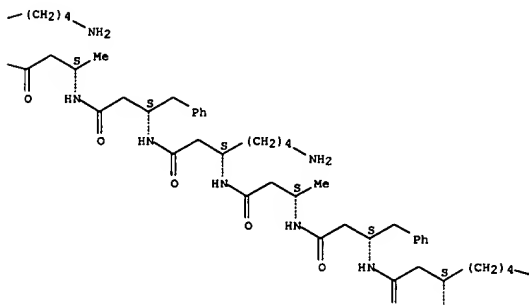
PAGE 1-A



PAGE 1-B



PAGE 1-C

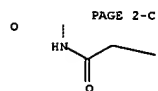


PAGE 1-D



PAGE 2-A

● 6 HCl



PAGE 2-D



RN 387339-23-3 CAPLUS
 CN 4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 44, 48, 52, 56, 60, 64, 68-
 Heptadecaazadoheptacontanoic acid, 71-amino-7, 19, 31, 43, 55, 67-hexakis (4-
 aminobutyl)-11, 23, 35, 47, 59-pentamethyl-5, 9, 13, 17, 21, 25, 29, 33, 37, 41, 45, 49, 5
 3, 57, 61, 65, 69-heptadecaazo-3, 15, 27, 39, 51, 63-hexakis (phenylmethyl)-,
 hexakis(trifluoroacetate) (9CI) (CA INDEX NAME)

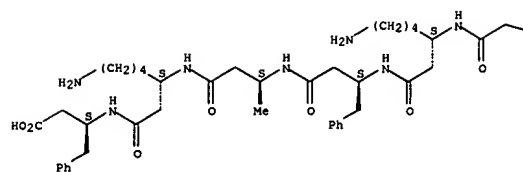
CM 1

CRN 387339-22-2

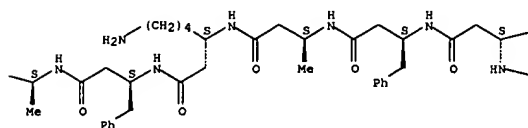
CMF C126 H194 N24 O19

Absolute stereochemistry.

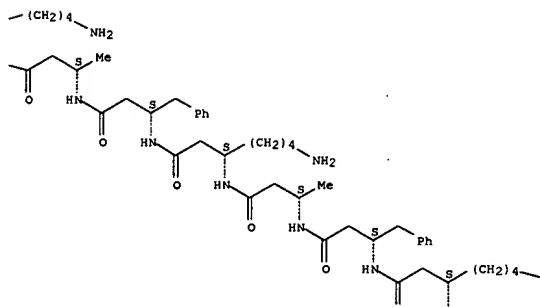
PAGE 1-A



PAGE 1-B

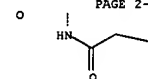


PAGE 1-C



PAGE 1-D

PAGE 2-C



PAGE 2-D



CM 2

CRN 76-05-1

CMF C2 H F3 O2

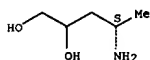


NH2

L12 ANSWER 39 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN
 AB Crotonaldehyde reacts with DNA to form two diastereomeric 1,N2 cyclic adducts of deoxyguanosine. A synthesis of the two diastereomeric deoxynucleosides has been achieved by reaction of mixed diastereomers of 4-amino-1,2-pentanediol with 2-fluoro-O6-(trimethylsilylethyl)-deoxyinosine. The resulting N2-(1-methyl-3,4-dihydroxybutyl)-deoxyguanosine was treated with NaIO4, cleaving the vicinal diol to the aldehyde. Spontaneous cyclization gave the two diastereomers of the crotonaldehyde-adducted nucleoside that were readily sepd. by HPLC. The abs. configurations were assigned by an enantiospecific synthesis of one diastereomer from (S)-3-aminobutanoic acid. The synthetic strategy has been extended to prep. of a site-specifically adducted oligonucleotide by reaction of the mixed diastereomers of 4-amino-1,2-pentanediol with an 8-mer oligonucleotide contg. 2-fluoro-O6-(trimethylsilylethyl)-deoxyinosine. The diastereomeric oligonucleotides were sepd. by HPLC and abs. configurations of the adducts were established by enzymic digestion to the adducted nucleosides.

ACCESSION NUMBER: 2001:748331 CAPLUS
 DOCUMENT NUMBER: 136:167616
 TITLE: Stereospecific Synthesis of Oligonucleotides Containing Crotonaldehyde Adducts of Deoxyguanosine
 AUTHOR(S): Nechev, Lubomir V.; Kozekov, Ivan; Harris, Constance M.; Harris, Thomas M.
 CORPORATE SOURCE: Department of Chemistry and Center in Molecular Toxicology, Vanderbilt University, Nashville, TN, 37235, USA
 SOURCE: Chemical Research in Toxicology (2001), 14(11), 1506-1512
 CODEN: CRTOEC; ISSN: 0893-228X
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:167616
 IT 381718-60-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (stereospecific synthesis of oligonucleotides contg. crotonaldehyde adducts of deoxyguanosine via cyclization of (dihydroxybutyl)deoxyguanosine)
 RN 381718-60-1 CAPLUS
 CN 1,2-Pentanediol, 4-amino-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L12 ANSWER 40 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)
 CRN 1565-74-8
 CMF C9 H12 O

Absolute stereochemistry. Rotation (+).



RN 389140-15-2 CAPLUS
 CN Benzenemethanol, .alpha.-ethyl-, (.alpha.R)-, compd. with (2S)-2-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 1565-74-8
 CMF C9 H12 O

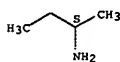
Absolute stereochemistry. Rotation (+).



CM 2

CRN 513-49-5
 CMF C4 H11 N

Absolute stereochemistry. Rotation (+).

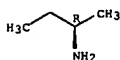


RN 389140-16-3 CAPLUS
 CN Benzenemethanol, .alpha.-methyl-, (.alpha.R)-, compd. with (2R)-2-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 13250-12-9
 CMF C4 H11 N

Absolute stereochemistry. Rotation (-).



L12 ANSWER 40 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN
 AB A methodol. has been developed for enantiodiscriminating chiral monoalcs. and monoamines by mass spectrometry. The approach is based on the generation of supersonically expanded complexes of these mols. with suitable chromophores, i.e. R-(+)-1-phenyl-ethanol (ER) or R-(+)-1-phenyl-1-propanol (PR). The jet-cooled diastereomeric complexes, otherwise elusive at room temp., have been ionized by one-color resonant two-photon absorption (R2PI) and their fragmentation pattern analyzed by time-of-flight (TOF) spectrometry. Enantiodifferentiation of the chiral monoalcs. and monoamines is based on: (1) the different spectral shifts of the band origin of their mol. complexes relative to that of the bare chromophore (.DELTA.) and (2) the different mass spectral fragmentation patterns of the jet-cooled diastereomeric adducts. Detection of stable aggregates of methane, n-butane, and other simple mols. with the selected chromophores suggests that the R2PI/TOF method can be a potential tool

for enantiodifferentiating chiral hydrocarbons in the gas phase.

ACCESSION NUMBER: 2001:746816 CAPLUS
 DOCUMENT NUMBER: 136:134373
 TITLE: Chiral discrimination of monofunctional alcohols and amines in the gas phase
 AUTHOR(S): Filippi, A.; Giardini, A.; Latini, A.; Piccirillo, S.; Scuderi, D.; Speranza, M.
 CORPORATE SOURCE: Dipartimento di Studi di Chimica e Tecnologia delle Sostanze Biologicamente Attive, Universita di Roma "La Sapienza", Rome, 00185, Italy
 SOURCE: International Journal of Mass Spectrometry (2001), 210/211(1-3), 483-488
 CODEN: IJMSFF; ISSN: 1387-3806
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

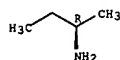
IT 389140-14-1 389140-15-2 389140-16-3
 389140-17-4
 RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
 (R2PI/TOF method for enantiodifferentiating chiral hydrocarbons in gas phase)

RN 389140-14-1 CAPLUS
 CN Benzenemethanol, .alpha.-ethyl-, (.alpha.R)-, compd. with (2R)-2-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 13250-12-9
 CMF C4 H11 N

Absolute stereochemistry. Rotation (-).



CM 2

L12 ANSWER 40 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN (Continued)

CM 2

CRN 1517-69-7
 CMF C8 H10 O

Absolute stereochemistry. Rotation (+).



RN 389140-17-4 CAPLUS
 CN Benzenemethanol, .alpha.-methyl-, (.alpha.R)-, compd. with (2S)-2-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 1517-69-7
 CMF C8 H10 O

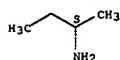
Absolute stereochemistry. Rotation (+).



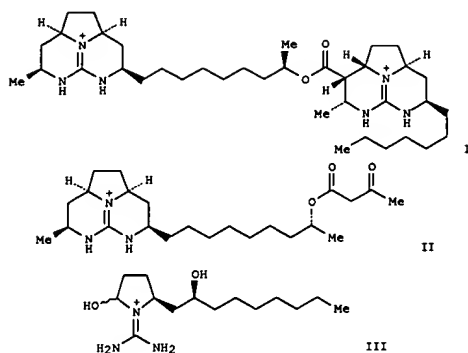
CM 2

CRN 513-49-5
 CMF C4 H11 N

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT



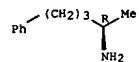
AB The first total synthesis of batzelladine F (I) as the bistrifluoroacetate salt was accomplished in 15 linear steps from two readily available enantiopure .beta.-hydroxy ketones. This enantioselective synthesis revises the structure of batzelladine F and defines its stereochem. Moreover, the scope of the tethered Biginelli condensation between .beta.-keto ester II as the BP4- salt and guanidine III as the acetate salt has been expanded to include the assembly of complex bisguanidines.

ACCESSION NUMBER: 2001:733456 CAPLUS
DOCUMENT NUMBER: 136:53928
TITLE: Enantioselective total synthesis of batzelladine F: structural revision and stereochemical definition
AUTHOR(S): Cohen, Frederick; Overman, Larry E.
CORPORATE SOURCE: Department of Chemistry, University of California, Irvine, CA, 92697-2025, USA
SOURCE: Journal of the American Chemical Society (2001), 123(43), 10782-10783
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 379668-87-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. total synthesis of batzelladine F via Biginelli condensation, its structure revision and stereochem.)
RN 379668-87-8 CAPLUS

L12 ANSWER 42 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN
AB Disubstituted nitroalkenes were converted into enantiomerically enriched amines (isolated as their hydrochloride salts) with enantiomeric excesses of 88 to >95% in three steps: (a) highly stereoselective conjugate addn. of the potassium salt of 4-phenyl-2-oxazolidinone; (b) radical-mediated removal of the nitro group; (c) cleavage of the oxazolidinone. The chiral amines thus prepd. included (+)-(2R)-2-butanamine hydrochloride, (-)-(.alpha.S)-.alpha.-ethylcyclohexanemethanamine hydrochloride, (+)-(.alpha.R)-.alpha.-methylbenzenebutanamine hydrochloride, (+)-(2R)-2-pentanamine hydrochloride, and (+)-(.alpha.S)-.alpha.-ethylbenzenepropanamine hydrochloride.

ACCESSION NUMBER: 2001:674597 CAPLUS
DOCUMENT NUMBER: 136:37082
TITLE: Enantioselective synthesis of .alpha.,.alpha.-disubstituted amines from nitroalkenes
AUTHOR(S): Leroux, M.-L.; Le Gall, T.; Mioskowski, C.
CORPORATE SOURCE: Service des Molecules Marquees, CEA-Saclay, Gif-sur-Yvette, 91191, Fr.
SOURCE: Tetrahedron: Asymmetry (2001), 12(13), 1817-1823
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 377080-82-5P, (+)-(.alpha.R)-.alpha.-Methylbenzenebutanamine hydrochloride
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of chiral amines via conjugate addn. of nitroalkenes to oxazolidinone and sequential redn. and ring opening of (nitroalkyl)oxazolidinones)
RN 377080-82-5 CAPLUS
CN Benzenebutanamine, .alpha.-methyl-, hydrochloride, (.alpha.R)- (9CI) (CA INDEX NAME)

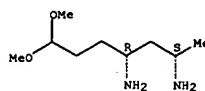
Absolute stereochemistry. Rotation (+).



● HCl

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

Absolute stereochemistry. Rotation (-).



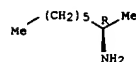
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

L12 ANSWER 43 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN
AB The reactions between di-Et N-(tert-butoxycarbonyl)phosphoramidate, diisopropyl azodicarboxylate (DIAD), triphenylphosphine (TPP) and primary or secondary alcs. lead to the corresponding di-Et N-alkyl-N-(t-butoxycarbonyl)phosphoramidates. Deprotection of crude intermediate in refluxing with p-toluenesulfonic acid monohydrate in ethanol affords ammonium tosylates in moderate to good overall yields. The N-alkylation of N-(tert-butoxycarbonyl)phosphoramidate proceeds stereoselectively with complete inversion of the configuration of the alkyl group.

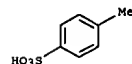
ACCESSION NUMBER: 2001:544538 CAPLUS
DOCUMENT NUMBER: 135:288324
TITLE: New protocol for converting alcohols into amines
AUTHOR(S): Klepacz, Anna; Zwierzak, Andrzej
CORPORATE SOURCE: Institute of Organic Chemistry, Technical University (Politechnika), Lodz, PL-90924, Pol.
SOURCE: Synthetic Communications (2001), 31(11), 1683-1689
CODEN: SYNCAN; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:288324
IT 365219-69-8P 365219-70-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of ammonium tosylates (amines) from alcs.)
RN 365219-69-8 CAPLUS
CN 2-Octanamine, (2R)-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1
CRN 34566-05-7
CMF C8 H19 N

Absolute stereochemistry.

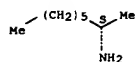


CM 2
CRN 104-15-4
CMF C7 H8 O3 S



RN 365219-70-1 CAPLUS
CN 2-Octanamine, (2S)-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)
CM 1
CRN 34566-04-6
CMF C8 H19 N

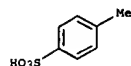
Absolute stereochemistry.



CM 2

CRN 104-15-4

CMF C7 H8 O3 S



REFERENCE COUNT:
THIS
FORMAT

13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR
RECORD. ALL CITATIONS AVAILABLE IN THE RE

AB .beta.-Peptides are a class of polyamides that have been demonstrated to adopt a variety of helical conformations. Recently, a series of amphiphilic L+2 helical .beta.-peptides were designed, which were intended

to mimic the overall physicochem. properties of a class of membrane-active

antimicrobial peptides, including magainin and cecropin. Although these peptides showed potent antimicrobial activity, they also showed significant activity against human erythrocytes. Operating under the assumption that their lack of specificity arose from excessive hydrophobicity, two addnl. .beta.-peptides H-(.beta.-3-HAla-.beta.-3-HLys-.beta.-3-HVal)n-NH2 (n = 4, 5) were designed and synthesized. Both have high antimicrobial activities, but very low hemolytic potencies. The peptides bind in an L+2 conformation to phospholipid vesicles, inducing leakage of entrapped small mol's. The peptides have a low affinity for membranes consisting of neutral phosphatidylcholine lipids, but bind avidly to vesicles contg. 10 mol % of acidic phosphatidylserine lipids. Differences in vesicle leakage kinetics for the two peptides suggest that chain length could affect their mechanisms of disrupting cell membranes. Thus, insights gained from the study of variants of natural

.alpha.-peptides have provided a useful guide for the design of nonnatural

antimicrobial .beta.-peptides.

ACCESSION NUMBER: 2001:514506 CAPLUS

DOCUMENT NUMBER: 135:257450

TITLE: De Novo Design, Synthesis, and Characterization of Antimicrobial .beta.-Peptides

AUTHOR(S): Liu, Dahui; DeGrado, William F.

CORPORATE SOURCE: Department of Biochemistry and Biophysics School of Medicine, University of Pennsylvania, Philadelphia, PA, 19104-6059, USA

SOURCE: Journal of the American Chemical Society (2001), 123(31), 7553-7559

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:257450

IT 361378-64-5P 361378-65-6P

RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL

(Biological study); PREP (Preparation)

(prepn., CD spectra, antimicrobial and membrane-binding activities of

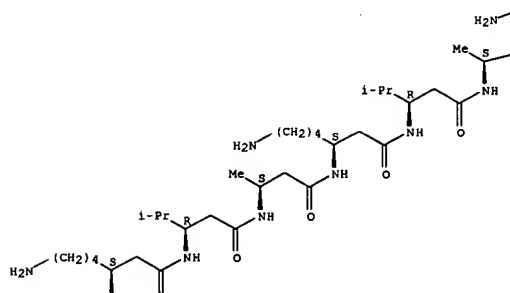
.beta.-peptides)

RN 361378-64-5 CAPLUS

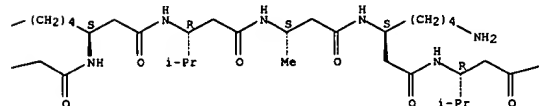
CN 4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 44, 48, 52, 56-Tetradecaazahexacontanamide, 47-amino-7, 19, 31, 43-tetrakis(4-aminobutyl)-11, 23, 35, 47-tetramethyl-3, 15, 27, 39, 51-pentakis(1-methylethyl)-5, 9, 13, 17, 21, 25, 29, 33, 37, 41, 45, 49, 53-tetrakis(1-methylethyl)-5, 9, 13, 17, 21, 25, 29, 33, 37, 41, 45-undecaazoo-, (3R, 7S, 11S, 15R, 19S, 23S, 27R, 31S, 35S, 39R, 43S, 47S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



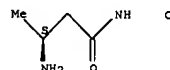
PAGE 1-B



PAGE 1-C

-NH2

PAGE 2-A



RN 361378-65-6 CAPLUS

CN 4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 44, 48, 52, 56-Tetradecaazahexacontanamide, 59-amino-7, 19, 31, 43, 55-pentakis(4-aminobutyl)-11, 23, 35, 47-tetramethyl-

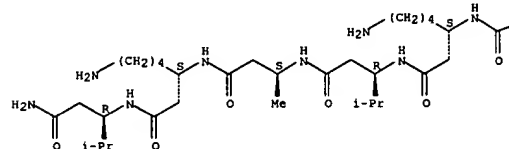
3, 15, 27, 39, 51-pentakis(1-methylethyl)-5, 9, 13, 17, 21, 25, 29, 33, 37, 41, 45, 49, 53

47-tetradecaazoo-, (3R, 7S, 11S, 15R, 19S, 23S, 27R, 31S, 35S, 39R, 43S, 47S, 51R, 55S,

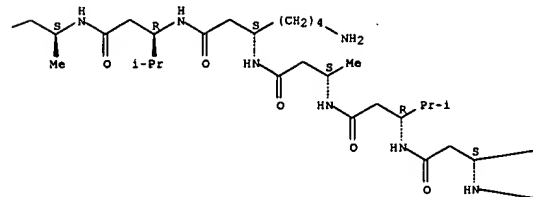
59S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

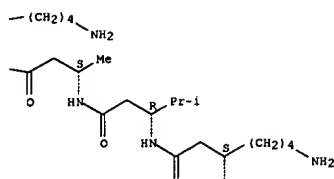
PAGE 1-A



PAGE 1-B



PAGE 1-C



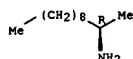
PAGE 2-C

REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L12 ANSWER 45 OF 45 CAPLUS COPYRIGHT 2003 ACS on STN
AB Chiral aliph. and arylalkyl amines are resolved in high enantiomeric excess (up to 97.5% ee for the R-enantiomers and up to 99.9% ee for the S-enantiomers) and good yield (50-80%) by using immobilized Candida antarctica lipase and Et acetate as acyl donor. A second resolin. on the R-amine increased the enantiomeric excess to more than 99.5% (up to 99.9%).

ACCESSION NUMBER: 2001:455215 CAPLUS
DOCUMENT NUMBER: 135:241912
TITLE: Resolution of chiral aliphatic and arylalkyl amines using immobilized Candida antarctica lipase and isolation of their R- and S-enantiomers
AUTHOR(S): Davis, Bruce A.; Durden, David A.
CORPORATE SOURCE: Neuropsychiatry Research Unit, University of Saskatchewan, Saskatoon, SK, S7N 5E4, Can.
SOURCE: Synthetic Communications (2001), 31(4), 569-578
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:241912
IT 360766-72-9P 360766-77-4P 360766-80-9P
360766-83-2P 360766-86-5P 360766-89-8P
360766-93-4P
RL: BFN (Biosynthetic preparation); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(resoln. of chiral aliph. and arylalkyl amines using immobilized Candida antarctica lipase)
RN 360766-72-9 CAPLUS
CN 2-Undecanamine, hydrochloride, (2R)- (9CI) (CA INDEX NAME)

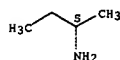
Absolute stereochemistry.



● HCl

RN 360766-77-4 CAPLUS
CN 2-Butanamine, (2S)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)
CM 1
CRN 513-49-5
CMF C4 H11 N

Absolute stereochemistry. Rotation (+).



CM 2

CRN 144-62-7
CMF C2 H2 O4



RN 360766-80-9 CAPLUS
CN 2-Pentanamine, (2S)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1
CRN 54542-13-1
CMF C5 H13 N

Absolute stereochemistry.



CM 2
CRN 144-62-7
CMF C2 H2 O4



RN 360766-83-2 CAPLUS
CN 2-Hexanamine, (2S)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1
CRN 70492-67-0
CMF C6 H15 N

Absolute stereochemistry. Rotation (+).



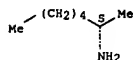
CM 2
CRN 144-62-7
CMF C2 H2 O4



RN 360766-86-5 CAPLUS
CN 2-Heptanamine, (2S)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1
CRN 44745-29-1
CMF C7 H17 N

Absolute stereochemistry. Rotation (+).



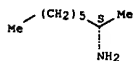
CM 2
CRN 144-62-7
CMF C2 H2 O4



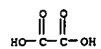
RN 360766-89-8 CAPLUS
CN 2-Octanamine, (2S)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1
CRN 34566-04-6
CMF C8 H19 N

Absolute stereochemistry.



CM 2
CRN 144-62-7
CMF C2 H2 O4

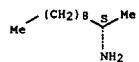


RN 360766-93-4 CAPLUS
CN 2-Undecanamine, (2S)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

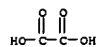
CRN 360766-92-3
CMF C11 H25 N

Absolute stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

=> fil caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
74.66	611.41

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-10.42	-42.97

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FILE COVERS 1907 - 5 Nov 2003 VOL 139 ISS 19
FILE LAST UPDATED: 4 Nov 2003 (20031104/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> fil reg
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.42	611.83

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-42.97

CA SUBSCRIBER PRICE

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STRUCTURE FILE UPDATES: 4 NOV 2003 HIGHEST RN 612801-40-8
DICTIONARY FILE UPDATES: 4 NOV 2003 HIGHEST RN 612801-40-8

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP

PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

Uploading 09857465.str

L13 STRUCTURE UPLOADED

=> d queyr

L13 HAS NO ANSWERS

'QUEYR ' IS NOT A VALID STRUCTURE FORMAT KEYWORD

Structure Formats

SIA ----- Structure Image, Attributes, and map table if it contains data. (Default)

SIM ----- Structure Image.

SAT ----- Structure ATtributes and map table if it contains data.

SCT ----- Structure Connection Table and map table if it contains data.

SDA ----- All Structure DATA (image, attributes, connection table and map table if it contains data).

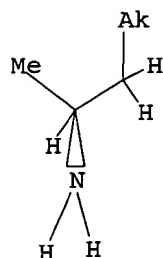
NOS ----- NO Structure data.

ENTER STRUCTURE FORMAT (SIM), NOS:nos

L13 STR

=> d query

L13 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l13

SAMPLE SEARCH INITIATED 16:57:22 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 141655 TO ITERATE

0.7% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000

PROJECTED ANSWERS: EXCEEDS 0

L14 0 SEA SSS SAM L13

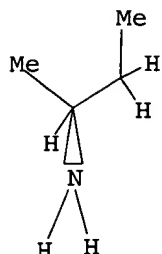
=>

Uploading 09857465.str

L15 STRUCTURE UPLOADED

=> d query

L15 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l15

SAMPLE SEARCH INITIATED 16:57:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 98610 TO ITERATE

1.0% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 0

L16 0 SEA SSS SAM L15

=> s l15 full

FULL SEARCH INITIATED 16:58:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 20.3% PROCESSED 400000 ITERATIONS 15 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.10

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
 BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 48

L17 15 SEA SSS FUL L15

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	148.55	760.38
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-42.97

FILE 'CAPLUS' ENTERED AT 16:58:16 ON 05 NOV 2003
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FILE COVERS 1907 - 5 Nov 2003 VOL 139 ISS 19
FILE LAST UPDATED: 4 Nov 2003 (20031104/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l17

L18 9 L17

=> d l18 8-9 abs ibib hitstr

L18 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS ON STN
AB A methodol. has been developed for enantiodiscriminating chiral monoalca. and monoamines by mass spectrometry. The approach is based on the generation of supersonically expanded complexes of these mols. with suitable chromophores, i.e. R-(+)-1-phenyl-ethanol (ER) or R-(+)-1-phenyl-1-propanol (PR). The jet-cooled diastereomeric complexes, otherwise elusive at room temp., have been ionized by one-color resonant two-photon absorption (R2PI) and their fragmentation pattern analyzed by time-of-flight (TOF) spectrometry. Enantiodifferentiation of the chiral monoalca. and monoamines is based on: (1) the different spectral shifts

of the band origin of their mol. complexes relative to that of the bare chromophore (.DELTA.) and (2) the different mass spectral fragmentation patterns of the jet-cooled diastereomeric adducts. Detection of stable aggregates of methane, n-butane, and other simple mols. with the selected chromophores suggests that the R2PI/TOF method can be a potential tool

for enantiodifferentiating chiral hydrocarbons in the gas phase.

ACCESSION NUMBER: 2001:746816 CAPLUS
DOCUMENT NUMBER: 136:134373
TITLE: Chiral discrimination of monofunctional alcohols and amines in the gas phase
AUTHOR(S): Filippi, A.; Giardini, A.; Latini, A.; Piccirillo, S.;
CORPORATE SOURCE: Scuderi, D.; Speranza, M.
Dipartimento di Studi di Chimica e Tecnologia delle Sostanze Biologicamente Attive, Universita di Roma

"La Sapienza", Rome, 00185, Italy
SOURCE: International Journal of Mass Spectrometry (2001), 210/211(1-3), 483-488
CODEN: IMSPFF; ISSN: 1387-3806
Elsevier Science B.V.

PUBLISHER: Journal
DOCUMENT TYPE: English
LANGUAGE: English

IT 389140-14-1 389140-15-2 389140-16-3
389140-17-4

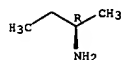
RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(R2PI/TOF method for enantiodifferentiating chiral hydrocarbons in gas phase)

RN 389140-14-1 CAPLUS
CN Benzenemethanol, .alpha.-ethyl-, (.alpha.R)-, compd. with (2R)-2-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 13250-12-9
CMF C4 H11 N

Absolute stereochemistry. Rotation (-).



CM 2

L18 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)

CM 2

CRN 1517-69-7
CMF C8 H10 O

Absolute stereochemistry. Rotation (+).



RN 389140-17-4 CAPLUS
CN Benzenemethanol, .alpha.-methyl-, (.alpha.R)-, compd. with (2S)-2-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 1517-69-7
CMF C8 H10 O

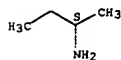
Absolute stereochemistry. Rotation (+).



CM 2

CRN 513-49-5
CMF C4 H11 N

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

L18 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2003 ACS ON STN (Continued)

CRN 1565-74-8
CMF C9 H12 O

Absolute stereochemistry. Rotation (+).



RN 389140-15-2 CAPLUS
CN Benzenemethanol, .alpha.-ethyl-, (.alpha.R)-, compd. with (2S)-2-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 1565-74-8
CMF C9 H12 O

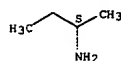
Absolute stereochemistry. Rotation (+).



CM 2

CRN 513-49-5
CMF C4 H11 N

Absolute stereochemistry. Rotation (+).

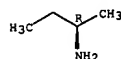


RN 389140-16-3 CAPLUS
CN Benzenemethanol, .alpha.-methyl-, (.alpha.R)-, compd. with (2R)-2-butanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 13250-12-9
CMF C4 H11 N

Absolute stereochemistry. Rotation (-).



L18 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2003 ACS ON STN

AB Chiral aliph. and arylalkyl amines are resolved in high enantiomeric excess (up to 97.5% ee for the R-enantiomers and up to 99.9% ee for the S-enantiomers) and good yield (50-80%) by using immobilized Candida antarctica lipase and Et acetate as acyl donor. A second resolu. on the R-amine increased the enantiomeric excess to more than 99.5% (up to 99.9%).

ACCESSION NUMBER: 2001:455215 CAPLUS
DOCUMENT NUMBER: 135:241912
TITLE: Resolution of chiral aliphatic and arylalkyl amines using immobilized Candida antarctica lipase and isolation of their R- and S-enantiomers
AUTHOR(S): Davis, Bruce A.; Durden, David A.
CORPORATE SOURCE: Neuropsychiatry Research Unit, University of Saskatchewan, Saskatoon, SK, S7N 5E4, Can.
SOURCE: Synthetic Communications (2001), 31(4), 569-578
CODEN: SYNCAR; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:241912

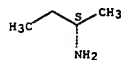
IT 360766-77-4P
RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(resolu. of chiral aliph. and arylalkyl amines using immobilized Candida antarctica lipase)

RN 360766-77-4 CAPLUS
CN 2-Butanamine, (2S)-, ethanediolate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 513-49-5
CMF C4 H11 N

Absolute stereochemistry. Rotation (+).



CM 2

CRN 144-62-7
CMF C2 H2 O4



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS
FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
9.49	769.87

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.30	-44.27

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FILE 'REGISTRY' ENTERED AT 16:59:01 ON 05 NOV 2003

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STRUCTURE FILE UPDATES: 4 NOV 2003 HIGHEST RN 612801-40-8

DICTIONARY FILE UPDATES: 4 NOV 2003 HIGHEST RN 612801-40-8

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

PROJECTED ITERATIONS: 3098 TO 4782
PROJECTED ANSWERS: 0 TO 0

L19 0 SEA EXA SAM L15

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.60	771.47

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-44.27

FILE 'CAPLUS' ENTERED AT 17:01:16 ON 05 NOV 2003
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```

=> s 360766-86-5/rn
      1 360766-86-5
      0 360766-86-5D
L24   1 360766-86-5/RN
      (360766-86-5 (NOTL) 360766-86-5D )

```

```

=> fil reg
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY      SESSION
FULL ESTIMATED COST          20.56      792.03

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                                ENTRY      SESSION
CA SUBSCRIBER PRICE          0.00      -44.27

```

FILE 'REGISTRY' ENTERED AT 17:06:11 ON 05 NOV 2003
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STRUCTURE FILE UPDATES: 4 NOV 2003 HIGHEST RN 612801-40-8
 DICTIONARY FILE UPDATES: 4 NOV 2003 HIGHEST RN 612801-40-8

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when

=> s 125

SAMPLE SEARCH INITIATED 17:06:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 98610 TO ITERATE

1.0% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 0

L26 0 SEA SSS SAM L25

=> logoff y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.40	792.43
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-44.27

STN INTERNATIONAL LOGOFF AT 17:06:30 ON 05 NOV 2003

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1204BXD

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 SEP 09 CA/CAPLUS records now contain indexing from 1907 to the
present
NEWS 4 AUG 05 New pricing for EUROPATFULL and PCTFULL effective
August 1, 2003
NEWS 5 AUG 13 Field Availability (/FA) field enhanced in BEILSTEIN
NEWS 6 AUG 18 Data available for download as a PDF in RDISCLOSURE
NEWS 7 AUG 18 Simultaneous left and right truncation added to PASCAL
NEWS 8 AUG 18 FROSTI and KOSMET enhanced with Simultaneous Left and Right
Truncation
NEWS 9 AUG 18 Simultaneous left and right truncation added to ANABSTR
NEWS 10 SEP 22 DIPPR file reloaded
NEWS 11 SEP 25 INPADOC: Legal Status data to be reloaded
NEWS 12 SEP 29 DISSABS now available on STN
NEWS 13 OCT 10 PCTFULL: Two new display fields added
NEWS 14 OCT 21 BIOSIS file reloaded and enhanced
NEWS 15 OCT 28 BIOSIS file segment of TOXCENTER reloaded and enhanced

NEWS EXPRESS OCTOBER 01 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

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of commercial gateways or other similar uses is prohibited and may
result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 17:51:45 ON 06 NOV 2003

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 17:51:52 ON 06 NOV 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file

provided by InfoChem.

STRUCTURE FILE UPDATES: 5 NOV 2003 HIGHEST RN 613214-61-2
DICTIONARY FILE UPDATES: 5 NOV 2003 HIGHEST RN 613214-61-2

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> s phenethylamine/cn

L1 1 PHENETHYLAMINE/CN

=> d l1

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 64-04-0 REGISTRY
 CN Benzeneethanamine (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Phenethylamine (8CI)
 OTHER NAMES:
 CN (.beta.-Aminoethyl)benzene
 CN (2-Aminoethyl)benzene
 CN .beta.-Phenethylamine
 CN .beta.-Phenylethylamine
 CN 1-Amino-2-phenylethane
 CN 2-Amino-1-phenylethane
 CN 2-Phenethylamine
 CN 2-Phenyl-1-ethylamine
 CN 2-Phenylethanamine
 CN 2-Phenylethylamine
 CN Ethanamine, 2-phenyl-
 CN NSC 10811
 CN O-PEA
 CN PEA
 FS 3D CONCORD
 MF C8 H11 N
 CI COM
 LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS,
 BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS,
 CHEMINFORMRX, CHEMLIST, CIN, CSCHM, DDFU, DETHERM*, DRUGU, EMBASE,
 GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*,
 MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA, PROMT, RTECS*, SPECINFO,
 SYNTHLINE,
 TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)

H₂N-CH₂-CH₂-Ph

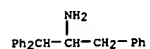
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6178 REFERENCES IN FILE CA (1907 TO DATE)
 296 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 6188 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> s 94964-58-6/rn
L2 1 94964-58-6/RN

=> d 12

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN 94964-58-6 REGISTRY
CN Phenethylamine, .alpha.-(diphenylmethyl)- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H21 N
CI COM
LC STN Files: CA, CAOLD, CAPLUS, CHEMCATS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> fil caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
8.38	8.59

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 17:53:10 ON 06 NOV 2003
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FILE COVERS 1907 - 6 Nov 2003 VOL 139 ISS 19
FILE LAST UPDATED: 5 Nov 2003 (20031105/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 94964-58-6/rn
1 94964-58-6
0 94964-58-6D
L3 1 94964-58-6/RN
(94964-58-6 (NOTL) 94964-58-6D)

=> fil beilstein
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
4.70	13.29

FULL ESTIMATED COST

FILE 'BEILSTEIN' ENTERED AT 17:54:54 ON 06 NOV 2003
COPYRIGHT (c) 2003 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften
licensed to Beilstein Chemiedaten & Software GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON OCTOBER 6, 2003

FILE COVERS 1771 TO 2003.
*** FILE CONTAINS 8,773,291 SUBSTANCES ***

>>> PLEASE NOTE: Reaction data and substance data are stored in separate documents and can not be searched together in one query.
Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a molecular formula or a structure search for example can be restricted to compounds with available reaction information by concatenation with PRE/FA, REA/FA or more general with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions.

For more detailed reaction searches BRNs can be selected from substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

```
*****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.          *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE      *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                    *
* FOR PRICE INFORMATION SEE HELP COST                             *
*****
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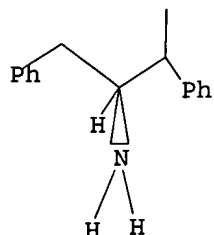
=>

Uploading 09857465.str

L4 STRUCTURE UPLOADED

=> d query

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 17:55:16 FILE 'BEILSTEIN'
SAMPLE SCREEN SEARCH COMPLETED - 40 TO ITERATE

100.0% PROCESSED 40 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 421 TO 1179
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4 full

FULL SEARCH INITIATED 17:55:24 FILE 'BEILSTEIN'
FULL SCREEN SEARCH COMPLETED - 670 TO ITERATE

100.0% PROCESSED 670 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.05

L6

4 SEA SSS FUL L4

=> d l6 1-4 abs ibib hitstr

'ABS' IS NOT A VALID FORMAT FOR FILE 'BEILSTEIN'

'IBIB' IS NOT A VALID FORMAT FOR FILE 'BEILSTEIN'

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'BEILSTEIN'

The following are valid formats:

QRD ----- Query Related Data (IDE plus HIT)

IDE ----- Identification of Substance, plus Structure

ALL ----- All Display fields (Lengthy displaye)

CHE ----- Chemical Data

PHY ----- Physical Data

HIT ----- All fields containing hit terms

Hit terms will be highlighted in all IDE fields in the BEILSTEIN file

A maximum of 20 values are displayed in each single property field.

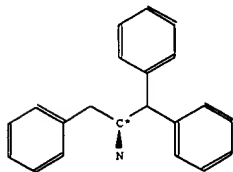
Use DISPLAY F<prop> for FULL format, e.g. FBP instead of BP.

For more information about display formats, and how to display individual selected properties, enter 'HELP FORMAT' at an arrow prompt, e.g. => HELP FORMAT.

ENTER DISPLAY FORMAT (QRD):ide

L6 ANSWER 1 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 8263040
 Autonom Name (AUN): 1-benzyl-2,2-diphenyl-ethylamine
 Molec. Formula (MF): C21 H21 N
 Molecular Weight (MW): 287.40
 Lawson Number (LN): 14414
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): isocyclic
 Constitution ID (CONSID): 7018224
 Tautomer ID (TAUTID): 7786001
 Entry Date (DED): 2000/03/03
 Update Date (DUPD): 2000/03/03



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2
ORP	Optical Rotatory Power	1

This substance also occurs in Reaction Documents:

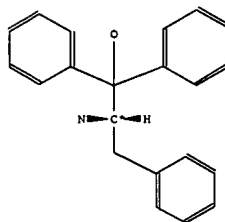
Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

L6 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 6120213
 CAS Reg. No. (RN): 23577-25-5, 100578-21-0
 Chemical Name (CN): (S)-2-amino-1,1,3-triphenyl-propan-1-ol;
 hydrochloride
 Frags. Molec. Formula (FMF): C21 H21 N O . Cl H
 Molecular Formula (MF): C21 H21 N O . Cl H
 Molecular Weight (MW): 303.40, 36.46
 Fragment BRN (FBRN): 3210568, 1098214
 Lawson Number (LN): 15135
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): isocyclic
 Constitution ID (CONSID): 5369162
 Tautomer ID (TAUTID): 5838998
 Beilstein Citation (BSO): 3-13-00-02080, 5-13
 Entry Date (DED): 1993/08/09
 Update Date (DUPD): 1994/11/08

CM 1

FBRN 3210568
 FMF C21 H21 N O



CM 2

FBRN 1098214
 FMF Cl H

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
RN	CAS Registry Number	2
CN	Chemical Name	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2

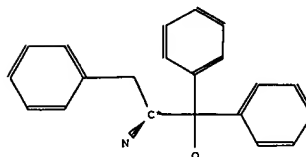
L6 ANSWER 2 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

(Continued)

Code	Name	Occurrence
FBRN	Fragment BRN	2
LN	Lawson Number	1
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	2
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	2

L6 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN): 5281434
 CAS Reg. No. (RN): 57728-37-7, 79868-78-3, 86906-05-0,
 126454-77-1
 Chemical Name (CN): (S)-2-amino-1,1,3-triphenylpropan-1-ol
 Autonom Name (AUN): 2-amino-1,1,3-triphenyl-propan-1-ol
 Molec. Formula (MF): C21 H21 N O
 Molecular Weight (MW): 303.40
 Lawson Number (LN): 15135
 File Segment (FS): Stereo compound
 Compound Type (CTYPE): isocyclic
 Beilstein Citation (BSO): 6-13
 Entry Date (DED): 1992/08/28
 Update Date (DUPD): 1992/08/30
 Compound Disposition (CDISP): 3210568 Alternate BRN



Fragment Notes:
 Stereo Descriptor: -

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
RN	CAS Registry Number	4
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
CDISP	Compound Disposition	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	1
ORP	Optical Rotatory Power	1
USC	Use of Compound	1

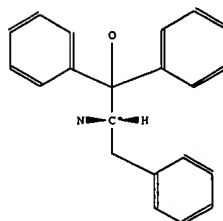
This substance also occurs in Reaction Documents:

L6 ANSWER 3 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

L6 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN

Beilstein Records (BRN):	3210568
CAS Reg. No. (RN):	57728-37-7, 79868-78-3, 86906-03-0, 126454-77-1
Chemical Name (CN):	(S)-2-amino-1,1,3-triphenyl-propanol- (1)
Autonom Name (AUN):	2-amino-1,1,3-triphenyl-propan-1-ol
Molec. Formula (MF):	C21 H21 N O
Molecular Weight (MW):	303.40
Lawson Number (LN):	15135
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	2667759
Tautomer ID (TAUTID):	3102397
Beilstein Citation (BSO):	5-13-00-00457, 3-13-00-02080, 5-13, 6-13
Entry Date (DED):	1990/02/15
Update Date (DUPD):	2001/10/25



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
RN	CAS Registry Number	4
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	1
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	4
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	3

L6 ANSWER 4 OF 4 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL on STN
(Continued)

NMR	Nuclear Magnetic Resonance	2
ORP	Optical Rotatory Power	4
RSTR	Related Structure	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	22
RXREA	Substance is Reaction Reactant	14
RXPRO	Substance is Reaction Product	8

=> logoff y
COST IN U.S. DOLLARS

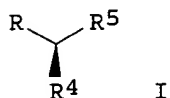
SINCE FILE	TOTAL
ENTRY	SESSION
33.78	47.07

FULL ESTIMATED COST

STN INTERNATIONAL LOGOFF AT 17:57:55 ON 06 NOV 2003

IONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 51 CAPLUS COPYRIGHT 2003 ACS on STN
GI



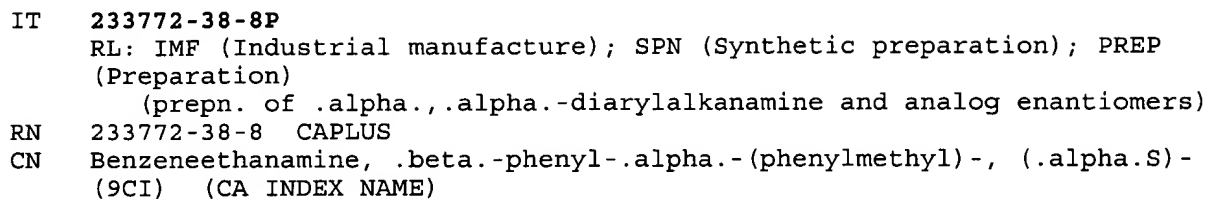
AB Title compds. [I; R = C(R2)3; R2 = H, (un)substituted alk(en)yl, etc.; R4 = e.g., NH2; R5 = C(R3)2R6; R3 = H, halo, alkyl, aryl, etc.; R6 = H or halo] were prepd. by treating I [R4R5 = e.g., NHCO2C(R3)2] with H or an H halide. Thus, (S)-Me2CHCH(NH2)CO2Me was treated with excess PhMgBr and the product cyclocondensed with ClCO2CCl3 to give (S)-I (R = CMe2, R4R5 = NHCO2CPh2) which was treated with H/Pd to give (S)-Me2CHCH(NH2)CHPh2.

ACCESSION NUMBER: 2000:401763 CAPLUS
DOCUMENT NUMBER: 133:43300
TITLE: Preparation of .alpha.,.alpha.-diarylalkanamine and analog enantiomers
INVENTOR(S): O'Hagan, David
PATENT ASSIGNEE(S): University of Durham, UK
SOURCE: PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000034210	A1	20000615	WO 1999-GB4031	19991206
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1135349	A1	20010926	EP 1999-959517	19991206
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRIORITY APPLN. INFO.:			GB 1998-26700	A 19981205
			WO 1999-GB4031	W 19991206
OTHER SOURCE(S): CASREACT 133:43300; MARPAT 133:43300				
IT 79868-78-3P				
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)				
(prepn. of .alpha.,.alpha.-diarylalkanamine and analog enantiomers)				
RN 79868-78-3 CAPLUS				
CN Benzenepropanol, .beta.-amino-.alpha.,.alpha.-diphenyl-, (.beta.S)- (9CI)				
(CA INDEX NAME)				

Absolute stereochemistry. Rotation (-).

instant

NC[C@H](S[C@@H](C1=CC=CC=C1)C2=CC=CC=C2)C3=CC=CC=C3

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT